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A Markov-Property Monte Carlo Method: One-Dimensional Ising Model

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In this paper we introduce a new Monte Carlo procedure based on the Markov property. This procedure is particularly well suited to massively parallel computation. We illustrate the method on the critical phenomena of the well known one-dimensional Ising model. In the course of this work we found that the autocorrelation time for the Metropolis Monte Carlo algorithm is closely given by the square of the correlation length. We find speedup factors of the order of 1 million for the method as implemented on the CM2 relative to a serial machine. Our procedure gives error estimates which are quite consistent with the observed deviations from the analytically known exact results.

KEY WORDS: Monte Carlo; Markov property; Ising model; critical phenomena.

1. INTRODUCTION AND SUMMARY

The purpose of this paper is to introduce a new method of acceleration for Monte Carlo calculations. It is specifically applicable to problems which possess the Markov property. We illustrate this method on the simple, well-known, one-dimensional, spin-1/2 Ising model. The usefulness of the method, of course, does not depend on the simple nature of this example. In our example we give exact analytic formulas for all the required quantities. From the operational point of view they simply yield a table of values and can be replaced with numerically obtained results in more complex models. Typically they can be computed once and for all at the beginning and simply stored, as we discuss in more detail below. In our example, the basic effect of the method is to replace the problem with a

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new problem which is effectively further from the critical point and so easier to compute.

A large class of important problems possess a key mathematical property called the Markov property. This property permits the introduction of new, specifically massively parallel, Monte Carlo methods to compute the solutions. The Markov property is simply stated. Consider a region $\mathscr{R}$ interior to a domain $\mathscr{D}$ over which a problem is stated. Let the problem variables on the boundary $\partial\mathscr{R}$ of $\mathscr{R}$ ($\partial\mathscr{R} \cap \mathscr{R} = \varnothing$) be fixed. This statement is meant to include values, and where appropriate, derivatives, etc. Then the problem is said to possess the Markov property if any expectation value of problem variables supported only in $\mathscr{R}$ is independent of all the problem variables supported in $\mathscr{D}\backslash(\mathscr{R} \cup \partial\mathscr{R})$. In the simple case of the one-dimensional Ising model, this definition means that if we fix the values of spins σ_i and σ_j, where $i<j$, so that we can define ($\partial\mathscr{R} = \{i, j\}$) $\mathscr{R} = \{k \mid i<k<j\}$, $\mathscr{D} = \{k \mid 1 \leqslant k \leqslant n\}$, then the partition function for this model becomes

$$
\begin{aligned}
Z &= \sum_{\substack{\sigma_k = \pm 1 \\ 1 \leqslant k \leqslant n \\ k \neq i, j}} \exp\left(K \sum_{k=1}^{n} \sigma_k \sigma_{k+1}\right) \\
&= \left[\sum_{\substack{\sigma_k = \pm 1 \\ k \in \mathscr{D}\backslash(\mathscr{R} \cup \partial\mathscr{R})}} \exp\left(K\sigma_j\sigma_{j+1} + K \sum_{k \in \mathscr{D}\backslash(\mathscr{R} \cup \partial\mathscr{R})}^{n} \sigma_k \sigma_{k+1}\right)\right] \\
&\quad \times \left[\sum_{\substack{\sigma_k = \pm 1 \\ k \in \mathscr{R}}} \exp\left(K\sigma_i\sigma_{i+1} + K \sum_{k \in \mathscr{R}} \sigma_k \sigma_{k+1}\right)\right] \qquad (1.1)
\end{aligned}
$$

In the case of periodic boundary conditions, we set $\sigma_{n+1} = \sigma_1$ and for free boundary conditions we set $\sigma_{n+1} = 0$. From the factorization of the partition function in (1.1) it is clear that the expectation value of any combination of spin variables supported in $\mathscr{R}$ depends only on the second factor and not at all on the first factor, since we are holding σ_i and σ_j fixed.

The Markov-property Monte Carlo method consists of exploiting this simple observation. It will be particularly useful for parallel computation. We remark that some previous use has been made of the simplest version of this property by dividing bipartite lattices into red and black vertices and summing in parallel over each color separately. The basic idea of our method is to divide the problem space up into a lot of small blocks which are separated from each other by a set of surfaces. That is to say, we break the problem up like a large mass of soap bubbles. We then fix the problem variables on the surfaces (soap bubbles) and sum over the blocks (interiors of the soap bubbles) in parallel. We then adjust the surface problem

variables by a Monte Carlo method. In the case of the one-dimensional Ising model which we will use to illustrate this technique, we break the n-spin system up into j blocks of $m+1$ spins $[n = j(m+1)]$. We then sum over the m interior spins in each block and adjust the remaining j spins by Monte Carlo. In general there is a choice as to how to do the summation over the spins which are in the interior. Since they depend only on boundary spin values, if the number of cases is not too numerous, it is clearly worthwhile to tabulate the results and not to have to recompute them at every step. In the case of the one-dimensional model there are just four cases: $(\uparrow\uparrow)$, $(\uparrow\downarrow)$, $(\downarrow\uparrow)$, and $(\downarrow\downarrow)$. Here we have simply computed the results analytically because of the simple nature of this problem. When the number of boundary cases is too numerous to tabulate, one can compute the sums over the block interiors directly in parallel, or one could perform a Monte Carlo computation on the interior of each block in parallel to obtain the results to adequate accuracy. Then the outer Monte Carlo procedures can be carried out on the surface problem variables. It is also sometimes useful to combine computation with tabulation so as to concatenate two smaller tables to give by a fairly quick computation results which are too large to be conveniently tabulated. For example, in the two-dimensional Ising model a 3×7 block has 16 nearest-neighbor spins or $2^{16} = 65{,}536$ boundary states. The equivalent of this table can be obtained by summing over the three spins (eight states) which join two 3×3 blocks each of which has eight nearest-neighbor spins or $2^8 = 256$ boundary states. This procedure is a further application of the Markov property.

More specifically, for our illustration, we use the following algorithm. First, set every $(m+1)$th spin. That is, set j of the spins to the value $+1$, where the total number of spins is $n = j(m+1)$. Second, sum over all possible values for the remaining jm spins. These spins can be divided into j blocks of m spins each, and the summation in each block is independent of that in all other blocks and so these summations can be performed in parallel. Since the one-dimensional Ising model is so simple, instead of having the computer do those sums, the results of which depend after all only on the values of the block-end-spins, we can give the necessary results for each of the statistics to be gathered by means of an analytic computation (see Section 2), but, as remarked above, for blocks of reasonable size even in more complex models, this information could have been directly numerically computed once at the beginning of the computation and simply tabulated. In any event, this organization of the work eliminates a great deal of redundant calculation! This second step gives one of the terms of the partially-summed partition function. This "new" partially-summed partition function is now thought of as a function of the remaining j spins alone. Third, make a Monte Carlo sweep over those j spins. We use the

simple Metropolis algorithm to do this sweep, and implement it by making a red–black dissection of those spins and then doing all spins of each color in parallel. Repeat the second and third steps until sufficient statistics have been gathered, with due attention, as detailed below, to the autocorrelation problem.

From the point of view of the statistical physics of critical phenomena, one outstanding unresolved problem revolves around the "renormalization group hypothesis."[1] By virtue of this hypothesis, all critical phenomena in a fixed spatial dimension, independent of the details of the atomic and molecular interactions, involving local variables of a given symmetry group exhibit a universal behavior. This universality means that it is only necessary to compute explicitly the behavior of one representative of each class, a considerable saving of effort. In the case of the three-dimensional Ising model, for example, the renormalization group hypothesis says that in the critical-point limit the Ising model corresponds to the same value of the renormalized coupling constant as does the strong-coupling limit of ϕ^4 boson field theory. There is some series and Monte Carlo evidence to suggest the contrary. A goal would be to develop a sufficiently powerful Monte Carlo procedure to be able to resolve this question clearly. We will therefore turn our attention in this paper toward the renormalized coupling constant for the one-dimensional Ising model.

In Section 2 we derive the necessary formulas for the one-dimensional Ising model. The situation for the case of periodic boundary conditions is fairly well known and the formulas are relatively simple. When the end spins of a block of spins are fixed and general, the results are not always known nor as simple to express. The breakdown of the required quantities into relevant independent parts and their evaluation is straightforward but tedious.

In Section 3 we begin the discussion of the application of our Monte Carlo procedure. Since the goal of this paper is to illustrate this method, we have used a simple Metropolis algorithm to perform the Monte Carlo part of the procedure. We find that the autocorrelation time for the magnetization is closely equal to the correlation length squared.

In Section 4 we give our Monte Carlo results. We have adopted the procedure of sampling only one sweep [spin update of the whole (Monte Carlo) lattice] per autocorrelation time. We set a goal to produce susceptibilities accurate to about 0.3%. A total of about 200,000 independent sweeps is sufficient to achieve this goal. We have broken them down into 40 coarse-grain samples of about 5000 each. This procedure is sufficient so that the error estimates computed on the basis of the coarse-grain data do not seem to differ in a statistically significant manner from the observed distribution of differences with the exactly known answers. Relative to a

serial machine, this method shows a speedup factor of $(m+1)^3$ times the number of parallel processors. This amounts to a factor of several million for some of the cases run. In terms of the dynamic critical exponent z the speedup factor $(m+1)^3$ becomes $(m+1)^{1+z}$.

2. FINITE-SIZE ONE-DIMENSIONAL ISING MODEL FORMULAS

In order to pursue the investigation of this method we need to derive a number of formulas for various quantities for a finite linear Ising chain[1] with the end spins fixed. This work is straightforward but rather tedious. We will in the main omit the derivations and comment only on the general approach for a specific result. In cases where it is impractical to compute these formulas analytically, they can usually instead be supplied numerically and the results tabulated. The goal is to compute the renormalized coupling constant.[2] It can be given by

$$\lim_{T \to T_c} g^*(K) = g^* \tag{2.1}$$

where $K = J/kT$, with J the exchange integral, T the temperature, k Boltzmann's constant, and where

$$g(K) = -\frac{v}{a^d} \frac{\partial^2 \chi(K)/\partial H^2}{\chi^2(K)\, \xi^d(K)} \tag{2.2}$$

with v the volume per unit cell, a the lattice spacing, and d the spatial dimension; $v = a$ and $d = 1$ here. We denote the magnetic field by H, the (reduced) magnetic susceptibility by χ, and the correlation length by ξ. It is convenient to note that we may write, for a chain of length n,

$$\chi(K) = \frac{1}{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \langle \sigma_j \sigma_k \rangle \tag{2.3}$$

$$\xi(K)^2 = \frac{1}{n} \left[\sum_{j=1}^{n} \sum_{k=1}^{n} (j-k)^2 \langle \sigma_j \sigma_k \rangle \right] \Big/ [2\chi(K)] \tag{2.4}$$

$$\frac{\partial^2 \chi}{\partial H^2} = \frac{1}{n} \sum_{j=1}^{n} \sum_{k=1}^{n} \sum_{l=1}^{n} \sum_{m=1}^{n} \langle \sigma_j \sigma_k \sigma_l \sigma_m \rangle - 3n[\chi(K)]^2 \tag{2.5}$$

and for the energy

$$\mathscr{E} = \frac{1}{n} \sum_{j=1}^{n} \langle \sigma_j \sigma_{j+1} \rangle \tag{2.6}$$

The notation $\langle \cdot \rangle$ means the unnormalized expectation value with respect to the partition function,

$$Z = \sum_{\sigma_j = \pm 1} \exp\left(K \sum_{j=1}^{n} \sigma_j \sigma_{j+1} \right) \tag{2.7}$$

where, by periodic boundary conditions, $\sigma_n \equiv \sigma_0$.

The strategy is now to break down the complete sum into blocks of $m+1$ spins each and to sum explicitly over the first m ($i = 1,..., m$) of the spins. We can always do this summation, independent of all the other spins in the system, because by the Markov property, only the $i = 0$ and $i = m+1$ spins have any effect on these sum values. This property can be seen directly from the Hamiltonian (2.7) in this simple case. Thus, for example, we can write, assuming that $n = (m+1)j$,

$$\left\langle \sum_{k=1}^{n} \sigma_k \right\rangle = \left\langle \sum_{l=1}^{j} \left[\left(\tfrac{1}{2}\sigma_{(l-1)(m+1)} + \sum_{\lambda=1}^{m} \langle \sigma_{(l-1)(m+1)+\lambda} \rangle_{\mathscr{C}_l} + \tfrac{1}{2}\sigma_{l(m+1)} \right) \prod_{\substack{i=1 \\ i \neq l}}^{j} \langle 1 \rangle_{\mathscr{C}_i} \right] \right\rangle_{\mathscr{B}} \tag{2.8}$$

where $\langle \cdot \rangle_{\mathscr{C}_l}$ is the constrained expectation value with respect to (2.7) within the lth block with all the $\sigma_{l(m+1)}$ fixed and the $\langle \cdot \rangle_{\mathscr{B}}$ is the remaining expectation value with respect to the j remaining spins. If we carry out these sums, we obtain

$$\begin{aligned} \langle 1 \rangle_{\mathscr{C}_l} &= (2\cosh K)^{m+1} \left(\tfrac{1}{2} + \tfrac{1}{2}\sigma_{(l-1)(m+1)}\sigma_{l(m+1)} \tanh^{m+1} K \right) \\ &= (\cosh^{(2m+2)} K - \sinh^{2m+2} K)^{1/2} \exp(K_m \sigma_{(l-1)(m+1)}\sigma_{l(m+1)}) \end{aligned} \tag{2.9}$$

$$\begin{aligned} &\tfrac{1}{2}\sigma_{(l-1)(m+1)} + \sum_{\lambda=1}^{m} \langle \sigma_{(l-1)(m+1)+\lambda} \rangle_{\mathscr{C}_l} + \tfrac{1}{2}\sigma_{l(m+1)} \\ &\quad = (2\cosh K)^{m+1} e^{2K} (1 - \tanh^{m+1} K) \tfrac{1}{4}(\sigma_{(l-1)(m+1)} + \sigma_{l(m+1)}) \end{aligned} \tag{2.10}$$

where we define K_m by

$$\exp(-2K_m) \equiv \frac{\cosh^{m+1} K - \sinh^{m+1} K}{\cosh^{m+1} K + \sinh^{m+1} K} \tag{2.11}$$

These equations can be derived by using the usual 2×2 matrix formalism for the one-dimensional Ising model. If we now compute the ratio of (2.10) to (2.9), we obtain the factor for

$$\begin{aligned} &\frac{1}{2}\sigma_{(l-1)(m+1)} + \sum_{\lambda=1}^{m} \langle \sigma_{(l-1)(m+1)+\lambda} \rangle_{\mathscr{C}_l} + \frac{1}{2}\sigma_{l(m+1)} \\ &\quad \hookrightarrow e^{2K} \left(\frac{1 - \tanh^{m+1} K}{1 + \tanh^{m+1} K} \right) \frac{1}{2} (\sigma_{(l-1)(m+1)} + \sigma_{l(m+1)}) \end{aligned} \tag{2.12}$$

to be used in Monte Carlo averages against the partition function when rewritten in terms of the nonexplicitly summed-over spins as

$$Z = 2^{mj}(\cosh^{2m} K - \sinh^{2m} K)^{j/2} \times \sum_{\sigma_{l(m+1)} = \pm 1} \exp\left(K_m \sum_{l=1}^{j} \sigma_{(l-1)(m+1)} \sigma_{l(m+1)} \right) \tag{2.13}$$

To obtain the formula for the susceptibility, when σ_j and σ_k of (2.3) are in different blocks, we can merely multiply the above results. When they are in the same block, we need the results for the factor for

$$\left\langle \left(\tfrac{1}{2}\sigma_{(l-1)(m+1)} + \sum_{\lambda=1}^{m} \sigma_{(l-1)(m+1)+\lambda} + \tfrac{1}{2}\sigma_{l(m+1)} \right)^2 \right\rangle_{\mathscr{C}_l}$$
$$\leftrightarrows -e^{4K}(1 - \sigma_{(l-1)(m+1)}\sigma_{l(m+1)}) + (m+1)\exp(2K - 2K_m \sigma_{(l-1)(m+1)}\sigma_{l(m+1)}) \tag{2.14}$$

This result seems most conveniently derived by diagonalization of the 2×2 matrix formulation in the presence of a magnetic field and then differentiating the results with respect to that field.

If we now add up these results, we get for the susceptibility

$$\chi = \frac{1}{n}\left\{ A(m, K) \left\langle \left(\sum_{l=1}^{j} \sigma_{l(m+1)} \right)^2 \right\rangle_{\mathscr{B}} + B(m, K) \left\langle \sum_{l=1}^{j} \sigma_{(l-1)(m+1)}\sigma_{l(m+1)} \right\rangle_{\mathscr{B}} + C(m, j, K) \right\} \tag{2.15}$$

where the coefficients are

$$A(m, K) = e^{4K}\left(\frac{1 - \tanh^{m+1} K}{1 + \tanh^{m+1} K} \right)^2$$
$$B(m, K) = -\frac{1}{2} A(m, K) + \frac{1}{2} e^{4K} - \frac{2(m+1)\, e^{2K} \tanh^{m+1} K}{1 - \tanh^{2m+2} K} \tag{2.16}$$
$$C(m, j, K) = (m+1)\, j e^{2K}\left(\frac{1 + \tanh^{2m+2} K}{1 - \tanh^{2m+2} K} \right) - \frac{1}{2} j[e^{4K} + A(m, K)]$$

and where the spins are distributed according to (2.11) and (2.13). Considerable use has been made of the periodic boundary conditions. We can also express the energy as

$$\mathscr{E} = D(m, K) + \frac{1}{j} E(m, K) \left\langle \sum_{l=1}^{j} \sigma_{(l-1)(m+1)}\sigma_{l(m+1)} \right\rangle_{\mathscr{B}} \tag{2.17}$$

where the coefficients are

$$D(m, K) = \frac{\tanh K - \tanh^{2m+1} K}{1 - \tanh^{2m+2} K}$$
$$E(m, K) = \frac{\tanh^m K(1 - \tanh^2 K)}{1 - \tanh^{2m+2} K} \tag{2.18}$$

In order to compute $\partial^2\chi/\partial h^2$, we will need to split up the quadruple sum in (2.5) into parts that are in the same block of $m+1$ spins and those which involve, by the Markov property, independent spins in different blocks. If we denote

$$S_l = \tfrac{1}{2}\sigma_{(l-1)(m+1)} + \sum_{\lambda=1}^{m} \sigma_{(l-1)(m+1)+\lambda} + \tfrac{1}{2}\sigma_{l(m+1)} \tag{2.19}$$

and

$$\left[\prod_{l \in \mathscr{L}} S_l\right] = \frac{\prod_{l \in \mathscr{L}} \langle S_l \rangle_{\mathscr{C}_l}}{\prod_{l \in \mathscr{L}} \langle 1 \rangle_{\mathscr{C}_l}} \tag{2.20}$$

then we want to divide

$$\begin{aligned}
&\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n}\sum_{m=1}^{n} \langle \sigma_j \sigma_k \sigma_l \sigma_m \rangle \\
&\quad = \sum_{j_1=1}^{j}\sum_{j_2=1}^{j}\sum_{j_3=1}^{j}\sum_{j_4=1}^{j} (1 - \delta_{12} + \delta_{12}) \\
&\qquad \times (1 - \delta_{13} + \delta_{13})(1 - \delta_{14} + \delta_{14})(1 - \delta_{23} + \delta_{23})(1 - \delta_{24} + \delta_{24}) \\
&\qquad \times (1 - \delta_{34} + \delta_{34})[S_{j_1} S_{j_2} S_{j_3} S_{j_4}] \\
&\quad = \sum_{j_1=1}^{j}\sum_{j_2=1}^{j}\sum_{j_3=1}^{j}\sum_{j_4=1}^{j} (1 - \delta_{12})(1 - \delta_{13}) \\
&\qquad \times (1 - \delta_{14})(1 - \delta_{23})(1 - \delta_{24})(1 - \delta_{34})[S_{j_1}][S_{j_2}][S_{j_3}][S_{j_4}] \\
&\qquad + 6(/) \sum_{j_2=1}^{j}\sum_{j_3=1}^{j}\sum_{j_4=1}^{j} (1 - \delta_{23})(1 - \delta_{24})(1 - \delta_{34})[S_{j_2}^2][S_{j_3}][S_{j_4}] \\
&\qquad + 3(//) \sum_{j_3=1}^{j}\sum_{j_4=1}^{j} (1 - \delta_{34})[S_{j_3}^2][S_{j_4}^2] \\
&\qquad + 4(\triangle) \sum_{j_3=1}^{j}\sum_{j_4=1}^{j} (1 - \delta_{34})[S_{j_3}^3][S_{j_4}] \\
&\qquad + (\oplus) \sum_{j_4=1}^{j} [S_{j_4}^4]
\end{aligned} \tag{2.21}$$

where the $\delta_{\mu\nu}$ are unity if $j_\nu = j_\mu$ and zero otherwise, and the diagrams in parentheses are the linear graphs which represent the term which follows, and the numerical coefficients are in fact the number of "strong" embeddings of that figure on the complete four-graph ($\oplus$) or tetrahedron. A strong embedding[3] is one for which nearest neighbors on the underlying graph must also be nearest neighbors on the unlabeled embedded graph. The other embeddings vanish because of the $(1-\delta)$ factors. In writing (2.21) use has been made of the identity $(1-\delta)^2 = (1-\delta)$. The expansion performed in (2.21) has served to give the results as sums over products of factors, each one of which is computed internal to a single block alone.

If we now expand the $(1-\delta)$ factors in (2.21), we obtain the required numerical coefficients as "weak" embeddings[3] on the appropriate underlying graph. A weak embedding is the number of ways an unlabeled graph fits on the unlabeled underlying graph. The resulting terms are simple sums over the j blocks. If we define the intermediate quantities

$$\begin{aligned}
&T_1 = \sum_{l=1}^{j} [S_l], \qquad T_2 = \sum_{l=1}^{j} [S_l^2], \qquad T_3 = \sum_{l=1}^{j} [S_l]^2 \\
&T_4 = \sum_{l=1}^{j} [S_l^3], \qquad T_5 = \sum_{l=1}^{j} [S_l][S_l^2], \qquad T_6 = \sum_{l=1}^{j} [S_l]^3 \\
&T_7 = \sum_{l=1}^{j} [S_l^4], \qquad T_8 = \sum_{l=1}^{j} [S_l^3][S_l], \qquad T_9 = \sum_{l=1}^{j} [S_l^2][S_l]^2 \\
&T_{10} = \sum_{l=1}^{j} [S_l^2]^2, \qquad T_{11} = \sum_{l=1}^{j} [S_l]^4
\end{aligned} \tag{2.22}$$

then we obtain from (2.21)

$$\begin{aligned}
&\sum_{j=1}^{n}\sum_{k=1}^{n}\sum_{l=1}^{n}\sum_{m=1}^{n} \langle \sigma_j \sigma_k \sigma_l \sigma_m \rangle \\
&\quad = T_1^4 - 6T_1^2 T_3 + 6T_1^2 T_2 - 6T_2 T_3 \\
&\qquad + 8T_1 T_6 - 12T_1 T_5 + 4T_1 T_4 + 3T_2^2 + 3T_3^2 - 6T_{11} \\
&\qquad + 12T_9 - 3T_{10} - 4T_8 + T_7
\end{aligned} \tag{2.23}$$

To make (2.22) fully explicit, we need the results

$$\begin{aligned}
[S_l] &= \tfrac{1}{2} C_1(m, K)(\sigma_{(l-1)(m+1)} + \sigma_{l(m+1)}) \\
[S_l^2] &= C_2(m, K) + D_2(m, K)\, \sigma_{(l-1)(m+1)} \sigma_{l(m+1)} \\
[S_l^3] &= \tfrac{1}{2} C_3(m, K)(\sigma_{(l-1)(m+1)} + \sigma_{l(m+1)}) \\
[S_l^4] &= C_4(m, K) + D_4(m, K)\, \sigma_{(l-1)(m+1)} \sigma_{l(m+1)}
\end{aligned} \tag{2.24}$$

where

$$C_1(m, K) = e^{2K}\left(\frac{1-\tanh^{m+1} K}{1+\tanh^{m+1} K}\right)$$

$$C_2(m, K) = -\frac{1}{2}e^{4K} + (m+1)\, e^{2K}\left(\frac{1+\tanh^{2m+2} K}{1-\tanh^{2m+2} K}\right)$$

$$D_2(m, K) = \frac{1}{2}e^{4K} - (m+1)\, e^{2K}\left(\frac{2\tanh^{m+1} K}{1-\tanh^{2m+2} K}\right)$$

$$C_3(m, K) = 3(m+1)\, e^{4K} + (e^{2K} - 3e^{6K})\left(\frac{1-\tanh^{m+1} K}{1+\tanh^{m+1} K}\right)$$

$$\begin{aligned} C_4(m, K) = {} & -2e^{4K} + \frac{9}{2}e^{8K} + 3(m+1)^2 e^{4K} \\ & + (m+1)\left[(e^{2K} - 6e^{6K})\left(\frac{1+\tanh^{2m+2} K}{1-\tanh^{2m+2} K}\right)\right. \\ & \left. - \frac{6e^{6K}\tanh^{m+1} K}{1-\tanh^{2m+2} K}\right] \end{aligned} \tag{2.25}$$

$$\begin{aligned} D_4(m, K) = {} & 2e^{4K} - \frac{9}{2}e^{8K} + (m+1)\left[3e^{6K}\left(\frac{1+\tanh^{2m+2} K}{1-\tanh^{2m+2} K}\right)\right. \\ & \left. + (12e^{6K} - 2e^{2K})\left(\frac{\tanh^{m+1} K}{1-\tanh^{2m+2} K}\right)\right] \end{aligned}$$

which are either drawn from those quoted above or derived by the method of differentiating with respect to the magnetic field as described above at (2.14). If we substitute (2.24) into (2.22) and the results into (2.23), we get, using (2.5),

$$\begin{aligned} \frac{\partial^2 \chi}{\partial H^2} = {} & [E_0(m, j, K) + E_1(m, K)\, Y_1(j, K_m) + E_2(m, j, K)\, Y_2(j, K_m) \\ & + E_3(m, K)\, Y_3(j, K_m) + E_4(m, j, K)\, Y_4(j, K_m) \\ & + E_5(m, K)\, Y_5(j, K_m)]/n - 3n[\chi(K)]^2 \end{aligned} \tag{2.26}$$

where

$$Y_1(j, K_m) = \left\langle \left(\sum_{l=1}^{j} \sigma_{l(m+1)} \right)^4 \right\rangle_{\mathscr{B}}$$

$$Y_2(j, K_m) = \left\langle \left(\sum_{l=1}^{j} \sigma_{l(m+1)} \right)^2 \right\rangle_{\mathscr{B}}$$

$$Y_3(j, K_m) = \left\langle \left(\sum_{l=1}^{j} \sigma_{l(m+1)} \right)^2 \sum_{l=1}^{j} \sigma_{(l-1)(m+1)} \sigma_{l(m+1)} \right\rangle_{\mathscr{B}}$$

$$Y_4(j, K_m) = \left\langle \sum_{l=1}^{j} \sigma_{(l-1)(m+1)} \sigma_{l(m+1)} \right\rangle_{\mathscr{B}}$$

$$Y_5(j, K_m) = \left\langle \left(\sum_{l=1}^{j} \sigma_{(l-1)(m+1)} \sigma_{l(m+1)} \right)^2 \right\rangle_{\mathscr{B}} \tag{2.27}$$

and also where

$$\begin{aligned}
E_0(m, j, K) &= -3C_1^2 C_2 j^2 + \tfrac{3}{4} C_1^4 j^2 + 3j^2 C_2^2 - 3C_1^4 j + 6C_1^2 (C_2 + D_2) j \\
&\quad - 3j(C_2^2 + D_2^2) - 2C_1 C_3 j + jC_4 \\
E_1(m, K) &= C_1^4 \\
E_2(m, j, K) &= -3jC_1^4 + 6jC_1^2 C_2 + 8C_1^4 - 12C_1^2 (C_2 + D_2) + 4C_1 C_3 \\
E_3(m, K) &= -3C_1^4 + 6C_1^2 D_2 \\
E_4(m, j, K) &= -3C_1^2 (C_2 + D_2) j + \tfrac{3}{2} C_1^4 j + 6jC_2 D_2 - 3C_1^4 \\
&\quad + 6C_1^2 (C_2 + D_2) - 6C_2 D_2 - 2C_1 C_3 + D_4 \\
E_5(m, K) &= -3C_1^2 D_2 + \tfrac{3}{4} C_1^4 + 3D_2^2
\end{aligned} \tag{2.28}$$

The final quantity that we need in order to compute the renormalized coupling constant is the correlation length. It can be derived[4] from the momentum-dependent susceptibility,

$$\begin{aligned}
\chi(n, k, K) &= \frac{1}{n} \sum_{r=1}^{n} \sum_{s=1}^{n} \exp[ika(r-s)] \langle \sigma_r \sigma_s \rangle \\
&= \sum_{j_1=1}^{j} \sum_{j_2=1}^{j} \exp\{ika[(j_1 - 1)(m+1) - (j_2 - 1)(m+1)]\} \\
&\quad \times \langle \mathscr{S}_{j_1}(k) \mathscr{S}_{j_2}^*(k) \rangle
\end{aligned} \tag{2.29}$$

where $i = \sqrt{-1}$, k is the momentum, and we define

$$\mathscr{S}_l(k) = \tfrac{1}{2} \sigma_{(l-1)(m+1)} + \sum_{r=1}^{m} e^{ikar} \sigma_{(l-1)(m+1)+r} + \tfrac{1}{2} e^{ika(m+1)} \sigma_{l(m+1)} \tag{2.30}$$

We require that $(nka/2\pi)$ be an integer. To compute (2.29) we will need the two basic ingredients $\langle \mathscr{S}_l \rangle_{\mathscr{C}_l}$ and $\langle |\mathscr{S}_l|^2 \rangle_{\mathscr{C}_l}$. For the first we get

$$\sum_{l=1}^{j} [\mathscr{S}_l(k)] = \mathscr{A}(m, k, K) \sum_{l=1}^{j} e^{ikal(m+1)} \sigma_{l(m+1)} \tag{2.31}$$

where $[\cdot]$ is as at (2.20) and

$$\mathscr{A}(m, k, K) = \mathrm{Re}[A_+ + A_- + (A_+ - A_-)\, e^{-ika(m+1)}] \tag{2.32}$$

with

$$A_+ = \frac{1}{2}\frac{(1+\tanh Ke^{ika})(1-\tanh^{m+1} K) + 2\tanh^{m+1} K(1-e^{ika(m+1)})}{(1-\tanh Ke^{ika})(1+\tanh^{m+1} K)}$$

$$A_- = \frac{1}{2}\frac{(1+\tanh Ke^{ika})(1-\tanh^{m+1} K) - 2\tanh^{m+1} K(1-e^{ika(m+1)})}{(1-\tanh Ke^{ika})(1+\tanh^{m+1} K)}$$

where $\mathrm{Re}[\cdot]$ stands for the real part. The factor to be averaged against the partition function (2.13) for the second ingredient is

$$\langle |\mathscr{S}_l|^2 \rangle_{\mathscr{C}_l} \hookrightarrow \hat{U}(m, k, K) + \hat{V}(m, k, K)\, \sigma_{(l-1)(m+1)}\sigma_{l(m+1)} \tag{2.33}$$

where

$$\begin{aligned}
\hat{U}(m, k, K) &= (m+1)\left(\frac{1+r^{2m+2}}{1-r^{2m+2}}\right)\left(\frac{1-r^2}{1+r^2-2r\cos ka}\right) + 1 \\
&\quad + \frac{2}{1-r^{2m+2}}\left(\frac{R_1 - r^{m+3}R_2}{(1+r^2-2r\cos(ka))^2}\right) \\
\hat{V}(m, k, K) &= \frac{-2(m+1)\, r^{m+1}(1-r^2)}{(1-r^{2m+2})(1+r^2-2r\cos(ka))} \\
&\quad + \frac{2}{1-r^{2m+2}}\left(\frac{r^2R_2 - r^{m+1}R_1}{(1+r^2-2r\cos(ka))^2}\right) \\
R_1 &= -1 + 2r\cos(ka) - r^2\cos(2ka) + r^{m+1}\cos(ka(m+1)) \\
&\quad - 2r^{m+2}\cos(kam) + r^{m+3}\cos(ka(m-1)) \\
R_2 &= \cos(ka(m-1)) - 2r\cos(kam) + r^2\cos(ka(m+1)) \\
&\quad - r^{m+1}\cos(2ka) + 2r^{m+2}\cos(ka) - r^{m+3}
\end{aligned} \tag{2.34}$$

where we use r as short for $\tanh K$ in these equations. If we combine these results, and remember to correct for the overlap terms in $|\sum_{l=1}^{j}[\mathscr{S}_l]|^2$, we obtain

$$\begin{aligned}
\chi(n, k, K) = \frac{1}{n}\Bigg\{ &|\mathscr{A}(m, k, K)|^2 \left\langle \left| \sum_{l=1}^{j} e^{ikal(m+1)}\sigma_{l(m+1)} \right|^2 \right\rangle_{\mathscr{B}} + jU(m, k, K) \\
&- jW(m, k, K) + [V(m, k, K) - X(m, k, K)] \\
&\times \left\langle \sum_{l=1}^{j} \sigma_{(l-1)(m+1)}\sigma_{l(m+1)} \right\rangle_{\mathscr{B}} \Bigg\}
\end{aligned} \tag{2.35}$$

where

$$
\begin{aligned}
U(m, k, K) &= \hat{U}(m, k, K) + \mathrm{Re}[A_+ + A_- + (A_+ - A_-)\, e^{-ika(m+1)}] - \tfrac{1}{2} \\
V(m, k, K) &= \hat{V}(m, k, K) + \mathrm{Re}[A_+ - A_- + (A_+ + A_-)\, e^{-ika(m+1)}] \\
&\quad - \tfrac{1}{2}\cos(ka(m+1)) \\
W(m, k, K) &= \tfrac{1}{2}\,|A_+ + e^{ika(m+1)}A_+^*|^2 + \tfrac{1}{2}\,|A_- - e^{ika(m+1)}A_-^*|^2 \\
X(m, k, K) &= \tfrac{1}{2}\,|A_+ + e^{ika(m+1)}A_+^*|^2 - \tfrac{1}{2}\,|A_- - e^{ika(m+1)}A_-^*|^2
\end{aligned}
\tag{2.36}
$$

Note that (2.35) reduces to (2.15) when $k = 0$.

There are a couple of useful expressions for the correlation length that we can derive from $\chi(n, k, K)$. The first is[4]

$$
\xi^2 = \frac{1}{4\sin^2(\frac{1}{2}ka)}\left(1 - \frac{\chi(n, k, K)}{\chi(n, 0, K)}\right) + O((ka)^2) \tag{2.37}
$$

where the best choice would be the smallest nonzero value for k, i.e., $ka = 2\pi/n$. Another expression is

$$
\begin{aligned}
\xi^2 = \Bigg[&\left(\frac{4\sin^2(\frac{1}{2}ka)\sin^2(ka)}{\sin^2(ka) - \sin^2(\frac{1}{2}ka)}\right) \\
&\times \left(\frac{1}{1 - \chi(n, k, K)/\chi(n, 0, K)} - \frac{1}{1 - \chi(n, 2k, K)/\chi(n, 0, K)}\right)\Bigg]^{-1}
\end{aligned}
\tag{2.38}
$$

which is exact for our model, the one-dimensional, n-spin Ising model with periodic boundary conditions, as the $\tanh^n K$ terms cancel out in

$$
1 - \frac{\chi(n, k, K)}{\chi(n, 0, K)} = \frac{4\tanh K \sin^2(\frac{1}{2}ka)}{1 + \tanh^2 K - 2\tanh K \cos ka} \tag{2.39}
$$

In order to check all these expressions, we note that they are in fact the exact renormalization group transformations for the decimation transformation[5] where m out of every $m+1$ spins are summed out. It is the case for the one-dimensional model that the space of Hamiltonians is unchanged under this transformation. Each such transformation corresponds to the map $K \mapsto K_m$, as given by (2.11). As a consequence, for any factorization of $n = j(m+1)$ we always arrive at the exact answer if we use the finite-size results for the j-spin, K_m system to complete what we have started by summing out the contributions from the m block-internal spins. We have programmed all these equations and compared a reasonable number of cases and find the expected agreement. Double precision (16 decimal places) was sometimes required because of the loss of accuracy involved in some of the expressions.

3. AUTOCORRELATION TIMES

In order to organize a Monte Carlo computation, it is desirable to have some idea of the correlation between the configurations found after one update (or sweep) of the entire spin lattice. Binder[6] suggests as a rough practical guide, which he justifies by discussions of the two- and three-dimensional Ising model, that the autocorrelation time diverges as the critical temperature is approached, like the static susceptibility. We will find that this suggestion is not correct in our case.

Since the purpose of this work is to study the improvement generated by block-internal summation of the interior spins, we have not used any of the more elaborate Monte Carlo methods available, such as the Swendsen–Wang[7] algorithms, but rather have used a straightforward Metropolis[8] algorithm. It is, of course, possible to combine the present method with more sophisticated methods than the Metropolis algorithm and one expects that the benefits from both will result in better results than those obtained from either method separately. As pointed out in the previous section, the decimaton transformation discussed maps the model onto a new Ising model with $K \mapsto K_m$ with the number of spins reduced by a factor of $(m+1)$. Thus we can divide the remaining linear array of j spins into those with an odd and those with an even site number. We can then try to flip, say all the odd ones, in parallel by the Markov property. If the sum of the nearest neighbor spins is zero, then the spin-flip probability is one-half. Otherwise the spin-flip probability is given by

$$p = \frac{\exp(K_m \sigma_i (\sigma_{i-1} + \sigma_{i+1}))}{2 \cosh 2K_m} \tag{3.1}$$

These calculations were done on the CM2 and were laid out to perform enough Monte Carlo calculations in parallel to keep the 512 floating point processors in one of the (quarter) partitions of the machine running at what is believed to be a relatively optimal ratio of virtual processors to physical processors.

Once the autocorrelation time has been found, the first ten autocorrelation time steps are discarded to avoid initial transients, and then only one configuration per autocorrelation time is sampled. The entire run is broken down into 40 coarse-grain samples for the purpose of later statistical analysis. The number of configurations sampled was chosen to achieve the desired final accuracy.

In order to calculate the autocorrelation time with any degree of accuracy, we aim to have a large enough gap between successive sample configuration so that the correlation coefficient is of the order of one-half. That is in contrast to, say, $r = 0.99$, where the random errors have a much

more significant effect on the estimate of the autocorrelation time. We began with the estimate of Binder mentioned above. We arbitrarily choose to look at 30 spin configurations (each separated from the previous one by the estimated autocorrelation time) for a coarse-grained sample. We then took a total of 40 close-grained samples. As the problem, as remarked above, again maps onto an Ising problem, we needed only to find the autocorrelation time as a function of K and system size. Since in the final analysis we wished to consider only systems which are free of finite-size effects to the 0.1 % level, the effect of system size disappears for sufficiently large systems, and leaves only K as an argument. We have computed the $M_t(K)\,M_{t+1}(K)$ and $E_t(K)\,E_{t+1}(K)$ correlation functions, where M is the magnetization and E the energy, and the time t is measured in units of the estimated autocorrelation time. We found, for the large autocorrelation times that occur as the temperature decreases toward zero (the critical temperature for this model), that the estimated autocorrelation began greatly to exceed that of the estimate. In a series of successive calculations, the estimate was increased until stability was achieved. Note that the autocorrelation time for the energy is noticeably shorter than that for the magnetization. Our final estimates are consistent with the result that the autocorrelation time for the Metropolis algorithm for the one-dimensional Ising model is just $1.00\xi^2$ with a statistical uncertainty of about 5 %.[2] The correlation length ξ for the infinite, linear-chain Ising model is given by

$$\xi^2 = \tfrac{1}{4}(e^{4K} - 1) \tag{3.2}$$

I am indebted to J. J. Erpenbeck for the simple argument that the penetration of a spin flip into a block of spins goes roughly at the rate of about $1/\xi$ per sweep, and it has to go a distance of ξ to decorrelate effectively, which leaves an autocorrelation time of the order of ξ^2. In the two-dimensional Ising model it is approximately true that ξ^2 diverges like the susceptibility χ [that is, $(1 - T_C/T)^{-1.75}$ versus $(1 - T_C/T)^{-2}$] and rather more closely so in three dimensions. Thus this result is not too different from Binder's suggestion in the latter two cases. The behavior of the autocorrelation time which we have found corresponds to a dynamical critical exponent of $z = 2$, which is quite a typical value in many problems for the Metropolis algorithm. Certainly, for some of the cluster algorithms, for example, z is much smaller, and if they were employed, since the critical slowing down would be less for those cases, the extra speedup factor attributable to this method would be correspondingly less.

[2] Note added: The exponent is exact; see ref. 9.

4. MONTE CARLO RESULTS

Near the critical point, which is zero temperature in our model ($K_c = \infty$), it is easy to estimate the asymptotic results for the autocorrelation times. From (2.11) we can compute that

$$\exp(-2K_m) \underset{K \to \infty}{\asymp} (m+1)\exp(-2K) \tag{4.1}$$

so by the results of Section 3, we get the autocorrelation time

$$\tau \approx \xi^2 \underset{K \to \infty}{\asymp} \frac{e^{4K}}{4(m+1)^2} \tag{4.2}$$

The formula (4.1) is exact for $m = 0$, as no summation takes place in that case. From (4.2) we see that there is a speedup factor of $(m+1)^2$. We note that using the same resources on a parallel machine, since there are a factor of $(m+1)$ fewer spins to sum over, we get an overall speedup factor of $(m+1)^3$ by running $(m+1)$ independent Monte Carlo runs in parallel. In addition we multiply by the number of parallel processors to give the appropriate comparison with a serial machine. For example, for $m = 15$ and using a quarter of the CM2 (512 floating point processors) we get a speedup of the order of 10^6. The reason for our choice of $m = 15$, rather than some other arbitrarily large number, is for comparison with what is possible when we do not have exact formulas available, as would be the case in more complex models. Here the number of states to be summed over is 32,768, which means it would have been completely feasible to generate the necessary coefficients by direct numerical summation. The next (power of two) case gives $m = 31$, or 2,147,483,648 states to sum over. Of course, for our model as explained above, we could get this case easily by concatenating two 16-spin blocks.

An illuminating table (very simple to construct) is Table I, which gives the correlation lengths (squared) as a function of block size $m+1$ and K

Table I. The Square of Correlation Length

K / $m+1 \backslash n$	0.5 / 16	1.0 / 64	1.5 / 128	2.0 / 512	2.5 / 1024	3.0 / 2048
1	1.6	13.4	100.6	745	5506	40688
2	0.35	3.3	25.1	186.2	1377	10172
4	0.05	0.76	6.2	46.5	344.1	2542.9
8	0.002	0.14	1.5	11.6	86	636
16		0.013	0.32	2.8	21.4	159

for the cases we will investigate. An added entry is the size n rounded to the next largest power of 2, which is needed to ensure that the finite-size effects are reduced to about 0.1 %.

In order to lay out our computations, we established the goal of a percentage error of around 0.3 % in the susceptibility. For our model, it is easy to give a theoretical estimate of the sum of the squares of the estimator for χ. It is directly given by the quadruple sum in (2.5). The dominant term in system size is just equal to the subtracted term, which is $3n^2\chi^2$. Straightforward calculation in this case shows the result to be independent of the size of χ (it scales out) and gives the conclusion that we need about 200,000 *independent* repetitions. As remarked above, we divide our samples into 40 coarse-grain samples for statistical purposes. Thus we aim to have about 5000 samples per coarse grain summary–that is, the number of sweeps per coarse-grain summary would be 5000 times the number in Table I. We have used a virtual processor ratio of 32 for efficiency on the CM2. That is, each physical processor is given 32 parallel cases to run, which reduces the startup computer overhead for each step. On this account and because of our organization so that all the parallel processors are kept equally busy, the actual number of repetitions per coarse-grain summary varies considerably, but is never less than 4096.

If we had run the case $K=3$ with a block size of unity, we would have needed about 1.7×10^{13} spin updates. This would have taken an estimated 500 hr to run with our code. This code is written in CM Fortran for the CM2, and has not been particularly streamlined for high performance, as that is not the point of this study. It runs at about 8×10^6 spin updates/sec on a quarter of the CM2, and could possibly be speeded up considerably by using Paris coding and the 16384-bit serial processors in a quarter of the CM2.

In order to assess the adequacy of our procedures, we have computed the temporal correlation coefficient between the estimate of the susceptibility in one coarse-grain sample and that for the next. The results for the cases we have run are listed in thousandths in Table II. We see that they are sufficiently small so that the error estimates (for χ certainly) will not be significantly affected by these correlations. In fact, since (neglecting finite-size effects) we compute that these correlations are expected to be $s/(m_2(1-s^2))$, where s is the sampled-sweep–sampled-sweep correlation and m_2 is the number of sampled sweeps per coarse-grain sample. For our case, $s\approx e^{-1}$ and $m_2\approx5000$. Thus the values in Table II should be about 10^{-4}. Consequently what we see is just the random errors of estimation about this much smaller value.

In order to be sure that our method is giving an accurate reflection of the errors, we need to compare the predicted errors with the actual errors,

Table II. Temporal Correlation Coefficient for the Susceptibility (in thousandths)

K	0.5	1.0	1.5	2.0	2.5	3.0
$m+1\backslash n$	16	64	128	512	1024	2048
1	3.8	−1.3	−3.1	−6.7		
2	1.3	2.1	3.2	2.9	−2.0	
4	−0.4	2.1	−0.04	1.9	1.1	
8	0.2	−0.8	5.9	1.7	−0.7	−3.8
16		−0.043	−7.4	−2.9	7.0	−0.4
32						1.9

as computed in terms of the known correct values. We make this comparison for the susceptibility in Table III. We have listed on the first line of each entry in Table III the actual errors (in percent) in the susceptibility χ estimated by our procedures as compared to the exact analytic results. The second line is the predicted root mean square error computed from the observed variance of the 40 coarse-grained samples.

There are several remarks to be made about Table III. First, the smaller numbers in the lower and left-hand portions of the table are due to our structuring the computer program to use all physical processor and to keep a virtual processor ratio of 32. These conditions mean that there is a minimum number of repetitions that we are set up to do. In the aforementioned instances, this minimum greatly exceeds the target number

Table III. The Error in the Estimated Susceptibility (in percent)

K	0.5	1.0	1.5	2.0	2.5	3.0
$m+1\backslash n$	16	64	128	512	1024	2048
1	0.2	0.06	−0.08	−0.5		
	0.22	0.31	0.31	0.31		
2	0.10	−0.2	0.06	0.3	0.09	
	0.16	0.32	0.32	0.27	0.31	
4	−0.01	0.6	−0.02	−0.1	−0.6	
	0.09	0.24	0.40	0.28	0.30	
8	0.01	0.1	0.1	0.4	−0.1	0.3
	0.03	0.18	0.31	0.31	0.31	0.29
16		0.02	0.01	0.1	−0.1	0.3
		0.06	0.18	0.40	0.34	0.32
32						0.3
						0.35

of 5000 per coarse-grained estimate. As there seemed no point in extra effort to throw out the additional repetitions, we kept them with the correspondingly better results. The next point to be noticed is that the errors are quite well in accord with the general predictions. Careful examination reveals that the estimates are, on average, larger than the true values by about 0.4 times the predicted error. The standard statistical chi-squared test on the square of the error over the square of the estimated error when applied to the data of Table III gives a result quite in line with expectations.

The statistical analysis of the other quantities which we are computing follows the same general pattern, but with different magnitudes for the errors. We will not report those in detail. We will discuss, however the estimation of the correlation length. The exact formula (2.38) is not sufficiently stable against random errors to be well adapted for Monte Carlo work. Instead we note, starting from (2.39), that

$$4\sin^2\left(\frac{1}{2}ka\right)\left(1-\frac{\chi(n,k,K)}{\chi(n,0,K)}\right)^{-1} = \frac{(1-\tanh K)^2+4\sin^2(\frac{1}{2}ka)\tanh K}{\tanh K} \tag{4.3}$$

which is a straight line in $4\sin^2(\frac{1}{2}ka)$ for our model, with unit slope and intercept ξ^{-2}. We have therefore used the average derived for the five lowest, nonzero momenta to estimate ξ^{-2}. We remind the reader that for our model, as we said in Section 2, there is no finite-size effect. In a formula like (2.37), the k^2 term would have a finite-size effect implicitly in it, as the smallest allowed k is of the order of $1/j$.

The errors in the energy are much smaller that those in the susceptibility. Those in the correlation length and the second partial of the susceptibility with respect to the magnetic field are larger. We illustrate these results in the typical case, $K=2.0$, $n=512$ with blocks of two spins ($m=1$). For this case we find

$$\begin{aligned} E &= 0.964080 \pm 0.000031 \quad (0.96402758) \\ \chi &= 54.78 \pm 0.15 \quad (54.598149) \\ \frac{\partial^2\chi}{\partial H^2} &= -4.810\times 10^5 \pm 9.6\times 10^3 \quad (-488209.64) \\ \xi^2 &= 750.6 \pm 9.8 \quad (744.98950) \end{aligned} \tag{4.4}$$

where the exact values are given in parentheses.

One of our important future goals would be the computation of the renormalized coupling constant in three spatial dimensions. For this reason

Table IV. The Error in the Estimated Renormalized Coupling Constant (in percent)

K	0.5	1.0	1.5	2.0	2.5	3.0
$m+1\backslash n$	16	64	128	512	1024	2048
1	0.2	−1.6	0.2	1.2		
	0.96	2.1	0.89	2.2		
2	0.4	−1.9	−1.3	−2.5	1.3	
	0.55	1.7	1.1	1.8	1.1	
4	0.03	−3.5	0.06	−0.8	−0.04	
	0.10	2.1	1.3	2.1	1.3	
8	0.003	1.0	−1.5	1.6	−1.9	−1.30
	0.012	1.0	0.85	2.0	1.2	0.72
16		−0.08	1.0	−3.5	1.7	0.3
		0.10	0.38	2.5	1.2	0.63
32						0.8
						0.69

we give our results in detail for the renormalized coupling constant. First, at the points $K=0.5$, 1.0, 1.5, 2.0, 2.5, and 3.0, the renormalized coupling constant has the values (for the system sizes listed in Table I) 6.1608036, 6.0187367, 6.0020793, 6.0003341, 5.9998893, and 5.9957266, respectively. It should be noted for our model that in the $n \to \infty$ limit, $g \geqslant 6$ for all K and $g \to 6$ as $K \to \infty$ for an infinite-size system. In Table IV we give the results in detail for the renormalized coupling constant g. Note that the errors are much larger here than in the case of the susceptibility. This reflects in large part the fact that the errors in $\partial^2\chi/\partial H^2$ are much larger than in χ because it is a four-point correlation function as opposed to a two-point correlation function, and the errors in ξ^2 are somewhat larger than in χ because of the effective subtraction of two two-point correlations necessary to derive it. The statistical χ^2 test shows that the observed actual errors (the first row in each category in Table IV) are consistent with the estimated errors (the second row in each category in Table IV). The conclusion is that this method of error estimation, the root mean square error estimate for the mean value from our 40 coarse-grained samples, is apparently a valid method of estimation for our case, where we have done our fine-grain sampling on sweeps separated by one temporal correlation length. The procedures we have adopted, i.e., 200,000 samples separated by a temporal correlation length and grouped into 40 coarse-grained samples, gives an estimate of g for our model accurate to within a standard error of around 2%.

Note that due to a bug in the CM2 operating system in time-sharing mode, sometimes incorrect results were produced. The author believes (hopes) that he has eliminated all such cases from this report.

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