

Some Monte Carlo Studies of the Ising Model

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Abstract The Markov property method of speeding up standard Monte Carlo methods can yield about an order of magnitude improvement for the two-dimensional Ising model. We also study the effects of finite size in the three-dimensional Ising model on the computation of the renormalized coupling constant and find, so long as the correlation length is less than about one-tenth the system width, that an accuracy of one percent or better can be expected.

1. Introduction

A critical-phenomena problem which remains unresolved is the proper analysis of the behavior of the renormalized coupling constant in the three-dimensional Ising model, and the attendant problems of the anomalous dimension of the vacuum, hyperscaling and universality. In this paper we report two studies which are intended to form a basis for an adequate numerical approach to the resolution of this problem. The first is the investigation of a Markov property method intended to speed up Monte Carlo simulations. It was introduced and tried on the one-dimensional Ising model by Baker [1]. Here we examine its effectiveness on the two-dimensional Ising model. We find that it can provide about an order of magnitude speedup in this case. Secondly we investigate in the three-dimensional Ising model the approach of the finite-system, renormalized coupling-constant, $g_r(K; L)$, to the infinite-system limit. We calculate values of $g_r(K; L)$ and the correlation length $\xi_L(K)$ for systems of width $L \leq 100$ by either Monte Carlo or exact summation. We find $(K/K_c)^{3/2}g_r(K; L)$ as a function of $\xi_L(K)/L$ to be approximately independent of L and that, for $\xi_L(K) < L/10$, $g_r(K; L)$ should agree with $g_r(K; \infty)$ to within at least one-percent.

2. Auto-Correlation Times in Two Dimensions.

In some previous work the idea was introduced [1] of using the Markov property

to speed up the Monte Carlo evaluation of thermodynamic functions in one dimension and to do [2] exact calculations on two-dimensional, finite-sized Ising model systems. In this section we extend the Markov-property, Monte-Carlo investigation to two dimensions. To remind the reader briefly, the Markov property means that for an Ising spin system, if we fix all the spins on the boundary of a finite region, then the expectation value of any function supported entirely in that region is completely independent of the spins outside that region. Baker [2] proposed the idea of dividing the plane-square lattice into diamond shaped regions, tabulating the sums of the appropriate quantities over all the interior spins of the diamonds as functions of the boundary-spin values, and then doing a Monte Carlo evaluation over the remaining boundary spins. Very significant speedups were obtained in one dimension [1].

In this study, we have considered four cases. The first case is meant to serve as a baseline and is the standard red-black decomposition of the lattice together with the standard Metropolis algorithm [3]. Since the purpose of this study is to consider the possible improvements due to block-internal spin summation, we use the straightforward Metropolis algorithm rather than a more sophisticated algorithm such as the Swendsen-Wang algorithm [4]. We used the Connection Machines routine “fast_rng” for the generation of the pseudo-random numbers. It is a lagged Fibonacci algorithm and we always used a 4 digit prime number as the initial seed. In this paper we use the term “auto-correlation time” to mean the number of “lattice updates” required so that the magnetization auto-correlation is equal to e^{-1} where e is the base of the natural logarithms. We denote this auto-correlation time by τ . By the term “lattice update” we mean that we apply the Metropolis algorithm once to each lattice spin to see if it should be flipped. In order to compute the auto-correlation time, we proceed as follows. Starting with a spin configuration, we perform a sufficient number, m , of lattice updates so that we estimate that the correlation between the magnetization at the original configuration and that in the new configuration to be about one-half. Typically our studies of the auto-correlation time were done with one sample taken every m lattice updates. Then 32 such sampled configurations were used in each of 40 coarse grain samples. These calculations were done on the CM-200. Some additional computations with 512 such sampled configurations for each of the 40 coarse grained samples were made on the CM-5. If the initial estimate and the observed auto-correlation times were too different, new estimates were used and the process continued until the estimate and the observations were fairly close. We have then computed the auto-correlation time by fitting a single exponential to the observed auto-correlation at a point where this auto-correlation is about one-half. This procedure yields estimates of the auto-correlation time which have statistical errors of about 2 - 3 percent which seems to be comparable to the accuracy claimed [5] for the same amount of computation for the sum of the observed auto-correlations over a window of time whose width is proportional to the auto-correlation time.

The second case studied was for the division of the spins of the plane-square

lattice into diamonds with 2 spins on each edge. They have 4 boundary spins and one interior spin. As explained above, this process is equivalent to picking a Monte Carlo configuration of the boundary spins and then summing the internal spins in each block to obtain the statistical weight of the boundary spin configuration. A comparison of the flipped and non-flipped configuration weights by means of the standard, Metropolis, asymmetric algorithm allows us to decide whether to accept or reject the spin-flipped configuration.

The third case divides up the plane into diamonds with 3 spins on each edge so that there are 8 boundary spins and 5 interior spins. The fourth case divides the plane up into diamonds with 5 spins on each edge so that there are 16 boundary spins and 25 internal spins in each diamond. The case of 4 spins on the edge was skipped because this division of the plane has a repeat distance of 6 which is not a power of two.

We have performed these calculations for a grid of about 8 inverse temperatures ranging over $0.1K_c \leq K \leq 0.975K_c$, where for the plane-square Ising model $K_c = 0.440686794\dots$. We have then fitted the auto-correlation times to a power law, with the most weight being given to the points closest to the critical temperature. We have obtained these results,

$$\begin{aligned}\tau_1 &\asymp 0.46(1 - K/K_c)^{-2.17}, \\ \tau_2 &\asymp 0.22(1 - K/K_c)^{-2.05}, \\ \tau_3 &\asymp 0.19(1 - K/K_c)^{-1.97}, \\ \tau_5 &\asymp 0.137(1 - K/K_c)^{-1.90},\end{aligned}\tag{2.1}$$

where the subscripts 1, 2, 3, 5 refer to the four cases described above. The dynamical scaling exponent, z is defined by $\tau = \xi^z$, where ξ is the spin-spin, correlation length. Since in the two-dimensional Ising model the correlation length exponent ν is exactly unity, as $\xi \propto (1 - K/K_c)^{-\nu}$ the exponents in (2.1) are direct estimates for the dynamical critical exponents in each of the above methods. The exponent z describes the ‘‘critical slowing down’’ in the sense that the length of the necessary Monte Carlo simulations for a given accuracy is proportional to the auto-correlation time which in turn is governed by z . The simulation time increases dramatically as the critical point is approached when z is large. By way of comparison, Stauffer [6] quotes the Monte Carlo result $z_1 = 2.17 \pm 0.01$, and Dammann and Reger [7] give the series result $z_1 = 2.183 \pm 0.005$.

In order to estimate the effectiveness of these procedures, we have run sample problems on 32 nodes of the CM-5. Since each node has four vector units attached to it, this configuration is effectively equivalent to 128 central processing units (cpus). This is to be contrasted with the 512 cpus used in our computations on the CM-200. We have used a trial problem where the inverse temperature is $0.9K_c$ on a 64×64 lattice for the basic problem. The number of lattice updates between the sampled configurations is as given by (2.1), and we have used 512 sampled configurations for each of the 40 coarse grained samples, as explained above. For this problem we have considered a mode where

we spread the problem across the machine and using all the nodes to process the problem in parallel, and the “idiot parallelization” mode, where 128 independent Monte Carlo problems (reducing the number of sample configurations per coarse grained step correspondingly) were run with each one running in a single cpu. For these parameters in cases 2 - 4, for the very same code, the idiot method was an order of magnitude faster on the CM-5 than the fully parallelized method, while in case 1 there was little time difference. For the trial problem we have found for case 1, 2381 seconds, for case 2, 1727, for case 3, 852, and for case 4, 267 seconds. Thus, the block-internal spin-summation method results in an order of magnitude improvement in the speed for the trial problem. The programs were all written in (Connection Machine) Fortran 90 in the same general style and no particular effort has been devoted to streamlining them as our current interest is in their relative speed.

A further set of parameters has been run for case 4 (the five-diamonds). A 256×256 lattice which has 16 times the number of spins in the trial problem was spread across the machine, but was run for only 32 repetitions for each of the 40 coarse grained samples. Since it was run for $K = 0.975K_c$, the number of lattice updates per sample is 151 instead of the 11 for the trial case. It required 7148 seconds which is roughly twice as long as would be expected in the idiot mode. Presumably for larger problems yet, the gap between the different modes will close further.

The computational times quoted in this section have been computed for comparability from actual cases which did not have exactly the proper number of skips between the sampled configurations.

3. Finite Size Behavior in Three Dimensions.

In a previous paper Baker [2] reported on the finite-size effects on the renormalized coupling-constant in two dimensions. The relevant thermodynamic function is,

$$g_r(K) = -\frac{v}{a^d} \frac{\frac{\partial^2 \chi(K)}{\partial H^2}}{\chi^2(K) \xi^d(K)}, \quad (3.1)$$

$$g^* = \lim_{K \rightarrow K_c^-} g_r(K), \quad (3.2)$$

where g^* is the renormalized coupling constant for the model. The quantity v is the volume of a unit cell on the lattice, a is the lattice spacing, χ is the susceptibility, H is the magnetic field, and d is the spatial dimension. The series results imply [8] that $g^* = 14.66 \pm 0.06$. In that paper [2] it was found that in two dimensions the value of $\lim_{L \rightarrow \infty} g_r(K_c; L)$ was less than about 3.1 while the values of $g_r(K; L)$ obtained for $K < K_c$ are very consistent with the series results for an infinite system, provided $\xi_L/L \leq 1/(7 \pm 1)$, where L is the

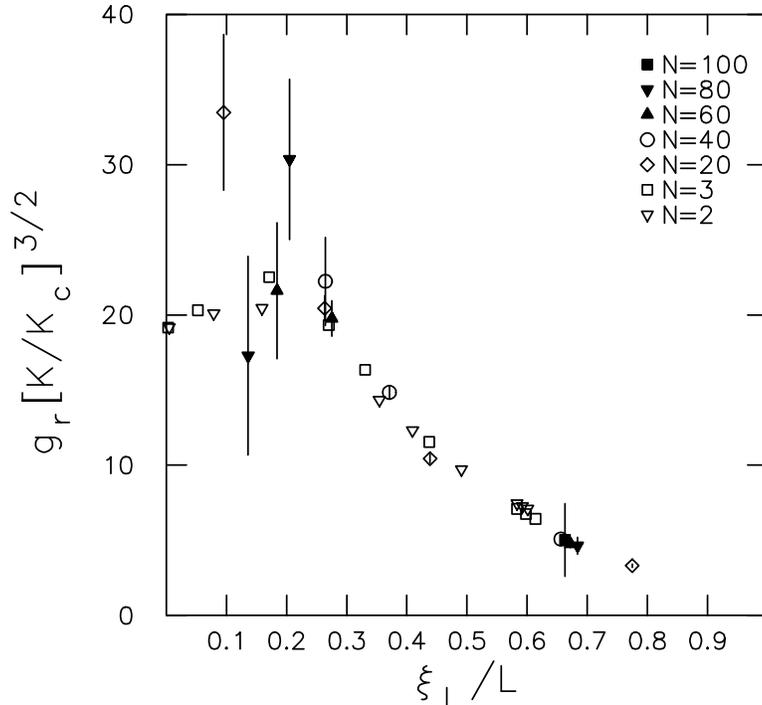


Fig. 1 Plot of $g_r(K; L)(K/K_c)^{3/2}$ for the three dimensional Ising model for simple cubic lattice systems of size $L \times L \times L$ spins versus $\xi_L(K)/L$. The point for $\xi_L = 0$ is common for all values of L .

system width. This difference was explained by analysis of finite-size effects. The correlation length was determined by fitting as parameters ξ_L^{-2} and A in,

$$4 \sum_{\omega=1}^d \sin^2\left(\frac{1}{2}\vec{q} \cdot \vec{e}_\omega\right) \left(1 - \frac{\chi(L^d, \vec{q}, K)}{\chi(L^d, \vec{0}, K)}\right)^{-1} = \xi_L^{-2} + A \sum_{\omega=1}^d \sin^2\left(\frac{1}{2}\vec{q} \cdot \vec{e}_\omega\right), \quad (3.3)$$

to the five smallest, non-zero values of \vec{q} allowed by periodic boundary conditions. Eq. (3.3) is exact with $A = 4$ for the one-dimensional Ising model.

It is of considerable interest to explore the finite-size behavior of $g_r(K; L)$ in three dimensions. To this end we have run a standard Monte Carlo code, (similar to that of Freedman and Baker [9]) on the CDC7600 for a very substantial period of time. Some of our results are displayed in Fig. 1, which shows the behavior of $g_r(K; L)$ when plotted against ξ_L/L . Results are given for $L = 2, 3, 20, 40, 60, 80, 100$. The results for $L = 2, 3$ are from exact summation and not Monte Carlo. The attention of the reader is drawn to the region of the plot where $\xi_L/L > \frac{1}{4}$. In this region we see very substantial data collapse, and it is in this region that we see that the finite-size effect is dominant. In the case of quantities which diverge, this finite-size effect is called finite-size rounding. In the simulation studies of the the three dimensional Ising model, it is also of interest to know how large a value of ξ_L/L can be used and still keep $|g_r(K; L)/g_r(K; \infty) - 1| < 0.01$, for example. {When K is not too close to K_c , $g_r(K; \infty)$ can be evaluated to adequate accuracy by series methods [8].}

For $L=2$, the answer is $\xi_2/2 \approx 0.08$ and for $L=3$, the answer is $\xi_3/3 \approx 0.11$. For the case $L = 20$, $K = 0.212$, we compute that $\xi_{20} = 5.26 \pm 0.03$ and for the case $L = 40$, $K = 0.215$ we compute that $\xi_{40} = 4.46 \pm 0.09$. Since the correlation length in this region of K is monotonic in K , it must be that for $L = 20$ and $K = 0.212$ that the finite-size, correlation-length value is well over a percent off the infinite-system value. Note is made that series analysis gives $\xi(0.212) \approx 3.6$. Thus $\xi_L/L = 0.26$ is too large for accurate work. This result represents a criticism of the work of Freedman and Baker [9] who used $\xi_L/L \approx 0.275$, and also of the work of a number of other workers. Series analysis is consistent with the above quoted results for $K = 0.215$, $L = 40$ within the errors of both analysis. Since the results for $L = 2, 3$ suggest that the allowed value of ξ_L/L increases with L , we think that the allowed value of ξ_L/L for large systems is somewhere between 0.11 and 0.26. The values $\xi_L/L \leq 0.10$ may very likely be safe for one-percent-level work.

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