PHYSICAL REVIEW

LETTERS

VOLUME 61 5 DECEMBER 1988 NUMBER 23

New Monte Carlo Technique for Studying Phase Transitions

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(Received 7 October 1988)

We present a new method for using the data from Monte Carlo simulations that can increase the efficiency by 2 or more orders of magnitude. A single Monte Carlo simulation is sufficient to obtain complete thermodynamic information over the entire scaling region near a phase transition. The accuracy of the method is demonstrated by comparison with exact results for the $d=2$ Ising model. New results for the $d=2$, eight-state Potts model are also presented. The method is generally applicable to statistical models and lattice gauge theories.

PACS numbers: 05.50.+q, 64.60.Fr, 75.10.Hk

Monte Carlo (MC) simulations have been used for many years to study the properties of physical models. A major concern for any thorough and accurate MC study is the amount of computer resources required. For large scale computations, such as those necessary to study lattice gauge theories,[1] the power and efficiency of the simulation are of major importance.

The desire to study larger and more complicated systems has been the impetus behind many advances in computation algorithms and computer hardware, aimed at increasing the speed at which a simulation is performed. Such advances have made it possible to study systems which would have been impossible to examine only a few years ago.

A different, but complementary approach to improving efficiency is to increase the amount of information obtained from a simulation. The data usually obtained from a MC simulation are averages of thermodynamic quantities at the single point in parameter space for which the simulation was performed. Early efforts to remove this limitation and obtain information over a range of parameters have had varying degrees of success.[2-4] Recently, Bhanot and co-workers[5-7] have made progress in this direction in calculations of the partition function of Z(2), Z(8), and SU(2) lattice gauge theories. Their technique uses multiple restricted-energy MC simulations to generate the partition function for a range of parameter values.

In this Letter, we present a related approach that is easier to implement, which uses standard simulation methods to generate continuous thermodynamic functions across the important region of parameter space. The data from a single simulation can be used, for instance, to study the entire scaling region near a phase transition, while with normal techniques, such a scan would require many simulations, producing a collection of individual points. Even three- or four-parameter scans, impossible to obtain with current simulation techniques, can be performed with this approach.

The method is especially important when the behavior of the system displays sharp peaks, such as near those near first- and second-order phase transitions, which are crucial for understanding the critical behavior of the model. Standard MC techniques locate the position of a narrow peak by multiple high-accuracy simulations. The result is a set of discrete points, none of which is exactly at the maximum. With the new technique, data from a single simulation can accurately locate the peak position and determine its height.

We demonstrate the reliability of this method by comparison with exact results for the $d=2$ Ising model. We demonstrate its power by performing the first calculation of exponentially small corrections to scaling at the first-order transition of an eight-state Potts model.

To illustrate the method, we consider a MC simulation of some physical model. Each configuration is generated

with its proper thermal weight. Time averages then give the equilibrium averages of any quantities of interest. These averages are the usual output of MC simulations. However, because the form of the probability distribution is known, it is possible to extract even more information from the simulation.

To see this, consider the Ising model in a magnetic field. The Hamiltonian for this system is

$$-\beta\mathcal{H} = K\sum_{\langle i,j\rangle}\sigma_i\sigma_j + h\sum_i \sigma_i = KS + hM ,$$

where K is the dimensionless coupling constant (J/kT) and h is an applied magnetic field (H/kT). The probability distribution of S and M at a point in the parameter space (K,h) is given by

$$P_{(K,h)}(S,M) = \frac{1}{Z(K,h)} N(S,M)\exp(KS+hM) , \quad (1)$$

where $N(S,M)$ is the number of configurations at the point (S,M) in the phase space, and $Z(K,h)$ is the canonical partition function given by

$$Z(K,h) = \sum_{S,M} N(S,M)\exp(KS+hM) .$$

The histogram of values of (S,M) generated by the MC simulation is proportional to $P_{(K,h)}(S,M)$. By storing this histogram on the computer, it is easy for one to generate the normalized probability distribution. The histogram can then be used to generate data for different parameters. The normalized probability distribution with new parameters (K',h') can be expressed in terms of the distribution with (K,h) in the following way:

$$P_{(K',h')}(S,M) = \frac{P_{(K,h)}(S,M)\exp[(K'-K)S+(h'-h)M]}{\sum_{S,M} P_{(K,h)}(S,M)\exp[(K'-K)S+(h'-h)M]} . \quad (2)$$

Since K' and h' are continuously variable, any quantities of interest can be calculated as continuous functions of the parameters. The denominator in Eq. (2) serves as an estimate for the partition function.[5-7]

This technique is easily generalized to other models, including those with continuous symmetry or more parameters.

To test the method, we performed MC simulations of the $d=2$ Ising model at the infinite-lattice transition temperature and zero magnetic field for lattice sizes $L=4$, 6, 8, 16, and 20. Between 4 and 6 million MC sweeps were performed for each lattice size with use of percolation representation algorithm due to Swendsen and Wang.[8] In Fig. 1, the calculated specific heat as a function of temperature is compared to the exact results[9] for $L=16$. Using these data, we were able to determine the position of the specific-heat maximum to within 0.04% and the value of the maximum to within 0.2%. Within the scaling region, the agreement between the MC results and the exact solution is excellent. For all

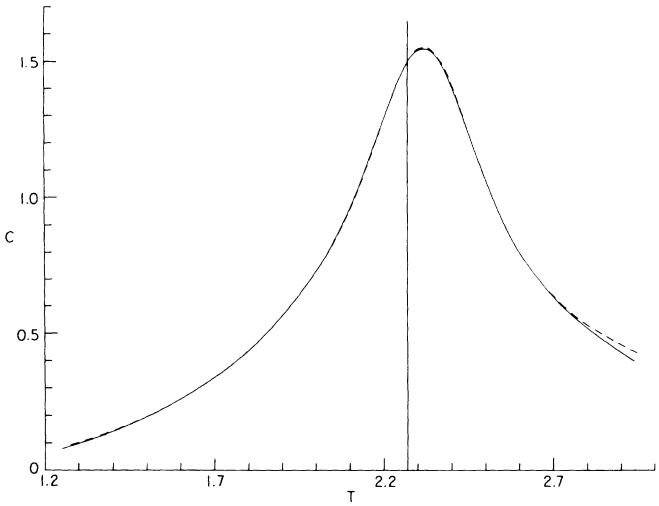

FIG. 1. Plot of specific heat vs T for the 16×16 $d=2$ Ising model. The dashed line is the exact solution (see Ref. 9) while the solid line is the result calculated from the single simulation at $T=T_c$. The location of the simulated temperature is marked with a vertical line.

temperatures in the range $T_c \pm 20\%$ the error is less than 0.5%.

The same MC data can also be used to study the Ising model below T_c in a magnetic field. In Fig. 2, the scaled magnetic susceptibility is shown plotted versus the scaled field for different sized lattices. The dashed line is the scaling curve predicted by Binder and Landau, who have studied finite size scaling at this first-order transition using standard MC techniques.[10] They performed multiple simulations for each lattice size using ~6 times as

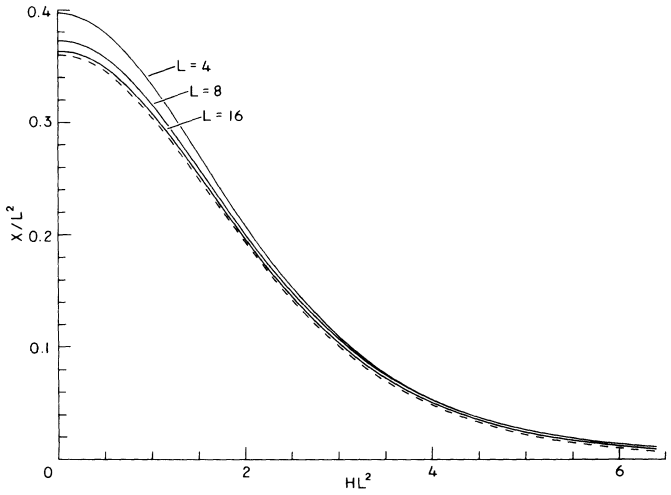

FIG. 2. Plot of scaled susceptibility vs scaled field for the $d=2$ Ising model at $T=2.1$. Results for $L=4$, 8, and 16 are shown. The dashed line is a scaling curve from Binder and Landau, Ref. 10. The data came from the same simulations as those used for Fig. 1.

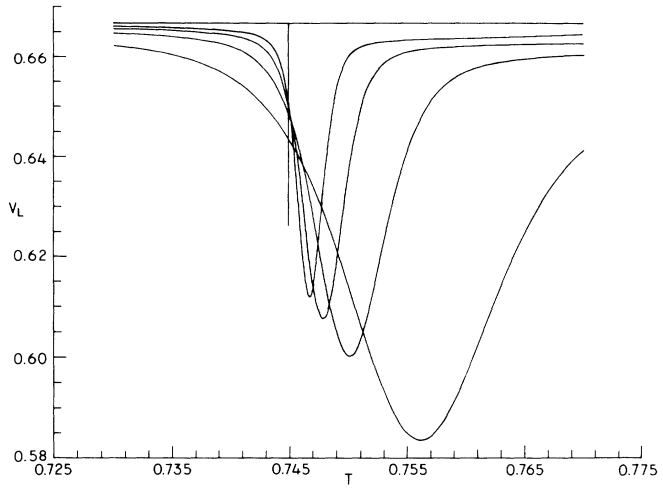

FIG. 3. Plot of Binder's reduced cumulant V_L vs temperature for the $d=2$, eight-state Potts model for $L=16$, 24, 32, and 40. The results are from single simulations at the finite lattice transition temperature. The infinite lattice limit for V_L (see Ref. 13) is also shown.

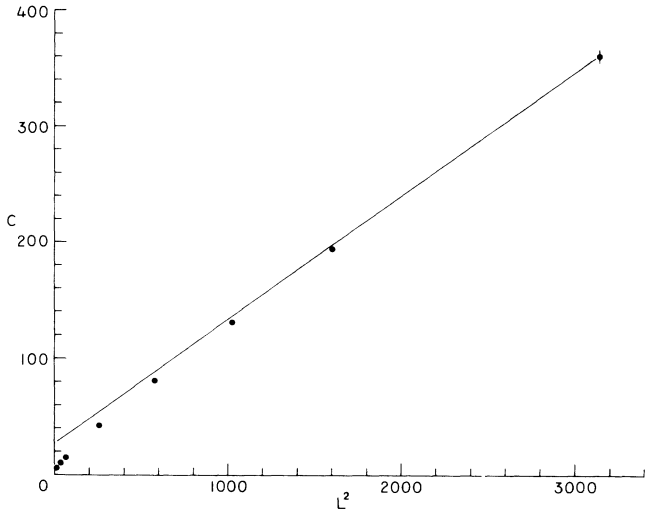

FIG. 4. Plot of the specific heat maximum vs L^2 for the $d=2$ eight-state Potts model for $L=4$, 6, 8, 16, 24, 32, 40, and 56. The data came from the same simulations as those used for Fig. 3. The solid line is the asymptotic scaling result.

much computer time as this study. The deviation from the scaling curve, also predicted by Binder and Landau, can clearly be seen. It should be emphasized that we obtained this field dependence from simulations in zero magnetic field and at a different temperature.

When we tested the method on the temperature-driven first-order phase transition in the $d=2$, eight-state Potts model,[11] the results were even better than expected. In practice, it can be extremely difficult to determine the order of a phase transition. The finite size of systems makes it impossible to see the discontinuities which characterize first-order transitions. Recently, Binder[12] has introduced a quantity that is very sensitive to the nature of a phase transition, but which requires a precise determination of the position and height of extremely narrow peaks. (For the first-order transition in the $d=2$, eight-state Potts model, the full-width of the peak for a 64^2 lattice is less than 0.2% of the transition temperature. In $d=3$, it is even narrower.) For the energy, this quantity, the reduced cumulant V_L, is defined by

$$V_L = 1 - \frac{\langle E^4 \rangle}{3\langle E^2 \rangle^2} .$$

At second-order transitions, $V_L \rightarrow \frac{2}{3}$ for all temperatures as $L \rightarrow \infty$. For the first-order transition in $d=2$ Potts models, V_L takes on the value $\frac{2}{3}$ for high and low temperatures, tending toward a known nontrivial value at the transition temperature.[13] For the eight-state Potts model, this value is 0.626 279 14 . . . .

We studied lattice sizes up to $L=56$ with simulations of up to 8×10^6 lattice sweeps. In Fig. 3, V_L calculated from simulation at T_c for each lattice size is shown plotted versus temperature. The location of the infinite lattice limit is also shown.

In Fig. 4, the specific heat maximum is shown plotted versus L^2. (The maximum scales with the volume of the system at a first-order transition.) The deviation from scaling can be clearly seen. For $d=2$ Potts models, the asymptotic behavior of the specific-heat maximum is known.[13] By subtracting the known scaling behavior, we were able to examine the corrections to scaling. We attempted fits to several types of functions, including power laws, but found that the data were best fitted with an exponential approach to a constant value. In Fig. 5, the corrections to scaling are shown along with the best

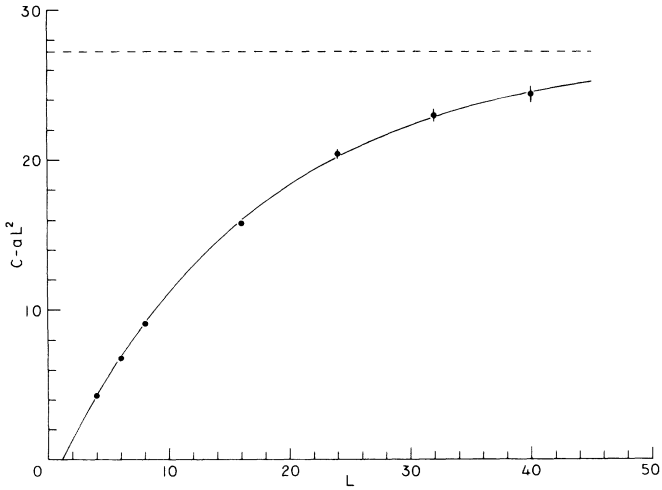

FIG. 5. Plot of the corrections to scaling vs L for the $d=2$, eight-state Potts model for $L=4$, 6, 8, 16, 24, 32, and 40. The data came from the same simulations as those used for Fig. 3. The solid line comes from a fit with Eq. (3) while the dashed line indicates the location of C_0.

fit with

$$C_{\max}(L) - aL^2 = C_0 + C_1 \exp(-L/l), \quad (3)$$

where l is related to the correlation length and a is related to the latent heat $\mathcal{L}$ by

$$a = \frac{\mathcal{L}^2}{4k_B T_c^2} = 0.1065739\ldots.$$

From the fit, we obtained the following values for the parameters:

$$C_0 = 27.7(4),$$

$$C_1 = 29.3(3),$$

$$l = 17.7(5).$$

The value of C_0 should be $\frac{1}{2}$ the sum of the specific heat of the ordered and disordered phases.[13] The values of the two specific heats can also be obtained by measurement of the second moments of the two peaks in the energy distribution. Using our results for $L = 56$, we estimate a value of C_0 of 26.5 ± 1.5 in agreement with the value obtained from the fit. A more detailed study of these corrections to scaling will be presented elsewhere.[14]

We have shown that this new technique can be used to greatly increase the amount of information extracted from a MC simulation at little cost in time or effort. (The results presented in this paper were obtained with Micro VAXII and Sun 3/52 workstations.) The ability to vary one or more parameters continuously makes the method useful in the study of systems with unknown or partially known behavior. In addition, this scanning ability simplifies and greatly improves the accuracy of the determination of the location and height of peaks of thermodynamic functions. This permits the study of scaling behavior, as well as an accurate determination of corrections to scaling. The technique is easily applied to other kinds of ensembles such as constant temperature or pressure molecular dynamics, microcanonical MC or quantum MC simulations, as well as for Monte Carlo renormalization-group calculations. The increase in efficiency (by 2 orders of magnitude or better) makes the method especially useful in the study of lattice gauge models, where large amounts of computer time are used. Because the partition function is also calculated (normalization of the probability distribution) the scanning technique can also be used for certain free-energy calculations. Thermodynamic functions can also be calculated at complex values of the temperature and fields making it possible to study the zeroes of the partition function in the neighborhood of the transition.[5-7]

We would like to thank K. Bassler, J. S. Wang, H. Park, and R. B. Griffiths for helpful discussions. This work was supported by National Science Foundation Grant No. DMR-8613218.

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