Sampling a Gaussian energy distribution to study the phase transitions of the $Z(2)$ and U(1) lattice gauge theories

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(Received 12 November 1986)

A new method for the study of phase transitions in classical statistical mechanics, by sampling a Gaussian energy distribution instead of a Boltzmann distribution, is applied to the $Z(2)$ and U(1) lattice gauge theories. The method is effective at identifying and measuring first-order transitions. The phase diagram of the U(1) gauge theory with both charge-1 and charge-2 interactions is described by this approach.

I. INTRODUCTION

The Monte Carlo method has been used with great success to study phase transitions in classical statistical mechanics.[1] The conventional technique is to generate an ensemble of states with the Boltzmann distribution $\exp(-\beta H)$, and to estimate the thermal average of any quantity $\langle Q \rangle$ at inverse temperature β by the ensemble average. A sharp change in $\langle Q \rangle$ as a function of β indicates the existence of a phase transition.

Although this method often yields good evidence of the existence of a phase transition, in some cases it does not yield accurate measurements of parameters of the transition such as the transition temperature or the latent heat. The reason is that the convergence of the Monte Carlo calculation is very slow near the phase transition. In the simulation of a large system the model may remain in a metastable supercooled or superheated phase, and this produces an error in the measurement. These metastable states create the phenomenon of hysteresis when making separate measurements for increasing and decreasing β. The transition temperature is uncertain by an amount comparable to the width in β of the hysteresis loop; the latent heat is uncertain by an amount comparable to the variation of $\langle H \rangle$ in the metastable state over the width of the loop.

Hysteresis is strongest in first-order phase transitions. Even second-order transitions will exhibit hysteresis if the number of Monte Carlo steps is sufficiently small. This occurs especially if the equilibrium states on either side of the transition differ significantly, requiring many Monte Carlo sweeps to bring the system from one state to the other. For such a system the usual Monte Carlo method may not even determine the order of the transition.

As an example of a system where it is important to measure accurately a first-order transition, consider the U(1) lattice gauge theory with action[2]

$$S=J_1\sum_p[1-\cos B(p)]+J_2\sum_p[1-\cos 2B(p)] \ . \quad (1.1)$$

Here let $\theta(l)$ be the U(1) gauge field at the link l; then $B(p)$ is the magnetic field at the plaquette p:

$$B(p)=\theta(l_1)+\theta(l_2)-\theta(l_3)-\theta(l_4) \ , \quad (1.2)$$

where the links l_1, l_2, l_3, l_4 form the plaquette p. We refer to the two terms in S proportional to J_1 and J_2 as charge-1 and charge-2 interactions. In a lattice gauge theory the action S plays the same role as the energy H in classical statistical mechanics. The phase diagram of the system described by Eq. (1.1) is shown in Fig. 1 for positive J_1 and J_2, where the axes β_1 and β_2 are

$$\beta_1=\beta J_1, \ \ \beta_2=\beta J_2 \ , \quad (1.3)$$

corresponding to inverse temperature β. The phase boundary AB is a second-order transition and the phase boundary from B toward increasing β_2 is a first-order transition. The order of the transition along the phase boundary BC is difficult to determine. For some distance along BC starting from B the transition is first order, but the latent heat decreases approaching C, and the transition appears to become second order at what may be a tricritical point (TCP) near C. The precise location of the TCP is not known. The first study of this model[2] indicated that the TCP has $\beta_2>0$ for a lattice of size 4^4. A re-

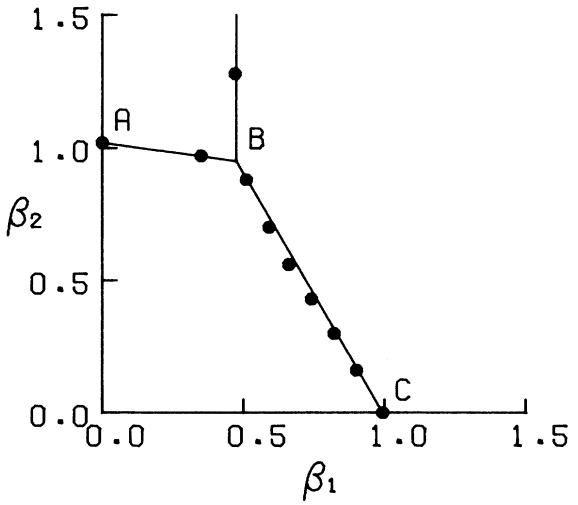

FIG. 1. The phase diagram of the U(1) lattice gauge theory with charge-1 and charge-2 interactions with coupling parameters β_1 and β_2, respectively.

cent more extensive study[3] suggests that for larger lattices the TCP has $\beta_2 < 0$; if so then the point C, i.e., the transition point of the simplest U(1) lattice gauge theory, with only charge-1 interactions, is a first-order transition. The fact that these and other calculations[4] have produced different evidence concerning the order of the transition at C shows why it is important to be able to measure the first-order transition accurately.

The purpose of this paper is to describe a new Monte Carlo approach to the study of phase transitions, as applied to the $Z(2)$ and U(1) lattice gauge theories in four dimensions. In this approach an ensemble is generated with a Gaussian energy distribution $\exp[-a(H-E_0)^2]$ rather than a Boltzmann distribution. The method has been applied previously to a phase transition in a system of classical spins, and is described briefly in a paper on that problem.[5] A more extensive discussion of the method is given in Sec. II of this paper. The lattice gauge theory calculations, described in Sec. III, are a strenuous test of the usefulness of this non-Boltzmann approach. The results indicate that this new method does yield accurate measurements of first-order phase transitions, and avoids the problem of hysteresis.

II. THE METHOD (REF. 6)

Derivation of the Boltzmann factor assumes an infinite heat bath in thermal contact with the system in question, total energy being conserved. We propose instead to connect the system to a *small thermometer* and to isolate the combined system. The exact properties of the thermometer are somewhat arbitrary but we will find it convenient to specify that its entropy be

$$S_\theta(E) = -aE^2 .$$

The negative value of S is permissible if we assume that the thermometer is a classical system. (Alternatively the thermometer could have been a quantum system but that would have required a careful attention to its density of states and the use of a less convenient form for the entropy.) If the system under study (hereafter called the sample) is in thermal contact with this thermometer then the entropy of the combined but isolated system is

$$S_{\text{tot}}(E) = \ln\rho(E) + S_\theta(E_0 - E) ,$$

where $\rho(E)$ is the sample's density of states, E_0 is the total energy of the combined system, E is the energy of the sample, and the difference is the energy of the thermometer. The average value of the energy of the sample is

$$\bar{E} = \int E \exp[S_{\text{tot}}(E)]dE \Big/ \int \exp[S_{\text{tot}}(E)]dE , \quad (2.1)$$

since the probability that the sample has energy E is proportional to the exponential of the total entropy. Because the thermometer is small we cannot use a linear approximation for the entropy as is done in the derivation of the Boltzmann factor but the thermometer entropy must be considered exactly. With the choice of the thermometer mentioned above Eq. (2.1) becomes

$$\bar{E} = \int E\rho(E)e^{-a(E-E_0)^2}dE \Big/ \int \rho(E)d^{-a(E-E_0)^2}dE . \quad (2.2)$$

To find the temperature of the thermometer we use the definition of $\beta = \partial S/\partial E$ for a general system and therefore for our thermometer

$$\beta \equiv \partial S_\theta/\partial E_\theta = -2aE_\theta = 2a(\bar{E} - E_0) . \quad (2.3)$$

This is the inverse temperature of the combined system when the sample has energy $\bar{E}$.

If one wants to proceed by simulation methods then the Metropolis method[7] is applied to the sampling function $\exp[-a(E-E_0)^2]$ where a is large enough that only a finite energy resides in the thermometer. (Some criteria for the choice of a are given below.) The calculation is performed for a series of E_0 and the resulting series of $\bar{E}$ and β are obtained, since $\bar{E}$ is just the average of E in the Metropolis ensemble and β is computed from Eq. (2.3). Using $\bar{E}$ instead of E_0 as the energy of the system amounts to subtracting off the energy of the thermometer.

This theoretical approach is now very close to the way many experiments are actually done. Consider a glass of ice water with a thermometer inserted. It is not connected to a heat bath at 0.0 °C but in fact is almost isolated from its environment. Heat energy is slowly diffusing into the glass from the environment and the ice-to-water ratio is changing as a result of the change of energy of the system including the thermometer. For a macroscopic system the temperature remains constant in the two-phase region of system energy. The state of the system is determined by the energy of the combined system of the ice water and thermometer.

When the system is not macroscopic the constancy of the temperature in the two-phase region is not required by thermodynamics. The proof of the equivalent statement that the entropy is convex (i.e., $\partial^2 S/\partial E^2 \leq 0$) requires the assumption that creation of the interphase surface does not carry an energy penalty. Thus for a small finite system the β vs $\bar{E}$ curve is s shaped in the transition region, as in Fig. 2. The criterion that the coexisting phases

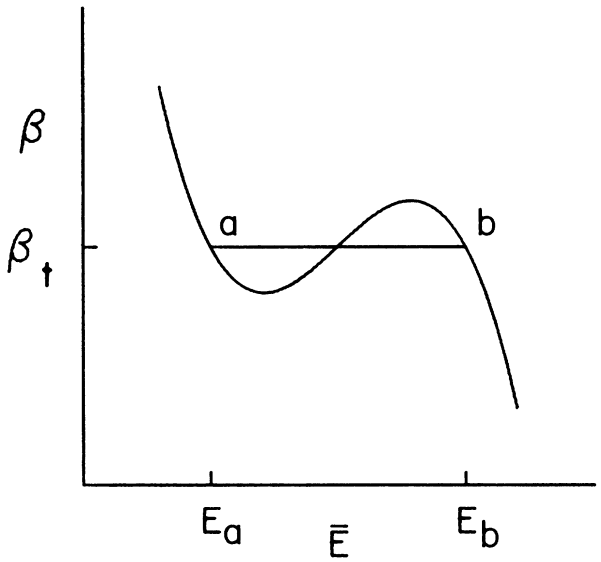

FIG. 2. The curve of β vs $\bar{E}$ in the region of a first-order phase transition. A finite system will follow the s-shaped curve in a transition between states a and b.

should have identical free energies and temperatures leads to an equal-area construction for the transition temperature as shown in the next paragraph.

The free energies of the two coexistent phases a and b at the transition temperature $1/\beta_t$ are

$$F = E_a - (1/\beta_t)S_a = E_b - (1/\beta_t)S_b \ ,$$

where E_a, E_b, and β_t are shown in Fig. 2 and where S_a and S_b are the entropies corresponding to the points a and b in Fig. 2. Multiplying by β_t and subtracting one has

$$(E_b - E_a)\beta_t - (S_b - S_a) = 0 \ . \tag{2.4}$$

By the definition of the temperature we obtain

$$S_b - S_a = \int_{E_a}^{E_b} \beta(E)dE \ .$$

Therefore the condition (2.4) can be written

$$\int_{E_a}^{E_b} [\beta(E) - \beta_t]dE = 0 \ . \tag{2.5}$$

Equation (2.5) is just the equal area criterion in the β,E plane similar to the more familiar one in the P,V plane.

The choice of the quantity a in Eq. (2.2) is important for the statistical error which will be observed. Large a corresponds to a small thermometer and therefore the thermometer's energy will fluctuate, decreasing the accuracy of the temperature measurement. Very small a corresponds to a large thermometer and in the limit will be no different than a heat bath. Some comments can be made about the choice of a between these extremes however.

The error in $\bar{E}$ and therefore in β is controlled by the distribution function

$$\exp[S_{\text{tot}}(E)]$$

which is approximately a Gaussian. The width of the Gaussian will depend on the second derivative of the total entropy. The standard deviation width σ of this Gaussian is

$$\sigma = 1/\sqrt{2a - \beta'} \ ,$$

where β' is the derivative of β with respect to energy. The error in β will be

$$\Delta\beta = 2a\Delta E \ ,$$

where ΔE is proportional to σ. Therefore the error in β is

$$\Delta\beta \propto a/\sqrt{2a - \beta'} \ .$$

If β' is positive (i.e., "inside" a first-order transition such as the region between a and b in Fig. 2) then a definite minimum of this function can be found by differentiation. The minimum is at

$$a = \beta' \ .$$

We have some preliminary confirmation of these effects on the statistical error.

Further exploration of the consequences of the assumption that the system is in equilibrium with a finite thermometer rather than a heat bath should prove interesting. The physical nature of the basis of the method, however, assures that all results will be satisfactory in the large-system limit.

III. LATTICE GAUGE THEORY CALCULATIONS

In this section we describe results of Monte Carlo calculations using the Metropolis method[1,7] to generate an ensemble of field configurations with a Gaussian probability distribution $\exp[-a(S - S_0)^2]$, where S is the action of a lattice gauge theory. [Remember not to confuse the action S and the entropy $S(E)$ discussed in Sec. II.] As derived in Sec. II, then the inverse temperature β is computed from $\langle S \rangle$, the mean value of S in the ensemble, by

$$\beta = 2a(\langle S \rangle - S_0) \ . \tag{3.1}$$

All the calculations are for a cubic lattice of dimension $5\times5\times5\times5$, with periodic boundary conditions. The parameter a of the Gaussian is rewritten as

$$a = \frac{1}{2\sigma^2 N_p{}^2} \ , \tag{3.2}$$

where N_p is the number of plaquettes, which is 3750 for the 5^4 lattice; the parameter σ, which will be called the Gaussian width, is a small number chosen such that the difference between $\langle S \rangle$ and S_0 is not large.

Figure 3 shows the average action *per plaquette* $\bar{S}$ vs β for the $Z(2)$ gauge theory, with action

$$S = \sum_p [1 - i(l_1)i(l_2)i(l_3)i(l_4)] \ , \tag{3.3}$$

where $i(l)$ is an Ising spin at link l. The points connected by line segments are computed by a conventional Metropolis Monte Carlo sampling of $\exp(-\beta S)$. The system was started in a random configuration, cooled by increasing β and then reheated by decreasing β, with 100 Metropolis sweeps between each change in β; the plotted points are

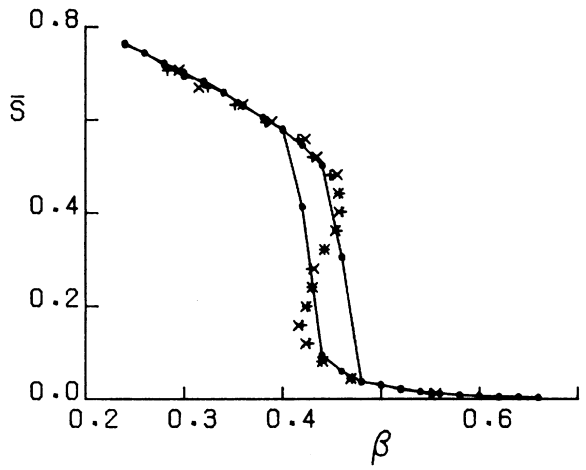

FIG. 3. Average action *per plaquette* $\bar{S}$ vs β for the $Z(2)$ gauge theory. The points connected by line segments are from sampling the Boltzmann distribution for both cooling and heating runs; the crosses ($+$ and $\times$) are from sampling the Gaussian distribution, with points plotted as $+$ and $\times$ for cooling and heating runs, respectively.

the averages of the last 50 of the 100 sweeps. The result shows the hysteresis produced by the first-order phase transition of the $Z(2)$ gauge theory. The other points, plotted as crosses ($\times$ and $+$), were computed by sampling the Gaussian energy distribution with $\sigma=0.005$. Again the system was started in a disordered configuration, and then cooled by decreasing S_0 and reheated by increasing S_0, with 200 Metropolis sweeps between each change in S_0; the $+$'s and $\times$'s, which are the averages of the last 150 of the 200 sweeps, were obtained during the cooling and heating runs, respectively. The results from the Gaussian distribution follow the Boltzmann hysteresis curves into the transition, where they form an s-shaped crossover, as expected according to the theory of the Gaussian distribution described in Sec. II. The amount of hysteresis in the Gaussian result is negligible. Therefore the equal-area construction explained in Sec. II gives a precise measurement of the transition: after averaging the cooling and heating runs the equal-area construction measures the transition temperature to be $\beta_t=0.439$, very close to the analytic value $\frac{1}{2}\ln(1+\sqrt{2})=0.440\,68$ known by the self-duality of the model. Also, the latent heat *per plaquette* is measured to be $S_b-S_a=0.423$, where S_a and S_b are the actions *per plaquette* at the end points of the equal-area construction. This calculation verifies that the Gaussian technique does accurately describe a first-order phase transition. It is also important to note that the Gaussian curve of $\bar{S}$ vs β follows the metastable states which are the origin of the hysteresis for the Boltzmann distribution, but does not itself have significant hysteresis.

The remaining calculations are for the U(1) gauge theory with both charge-1 and charge-2 interactions, for which the action S is defined in Eq. (1.1). The two coupling parameters β_1 and β_2 defined in Eq. (1.3) are rewritten as

$$\beta_1=\beta\cos\phi\ ,\qquad \beta_2=\beta\sin\phi\ , \tag{3.4}$$

where β is the inverse temperature and

$$\tan\phi=\frac{J_2}{J_1}\ ; \tag{3.5}$$

the angle ϕ is always given in terms of degrees. Figures 4 and 5 show results for $\phi=0°$ and 30°. The plotted points have the same meaning as in Fig. 3. The points connected by line segments are from sampling $\exp(-\beta S)$, and are the averages of the last 50 of 100 sweeps between each change in β; this produces a large hysteresis in both cases. The crosses ($+$'s and $\times$'s) are from sampling $\exp[-a(S-S_0)^2]$, and these are the averages of the last 150 of 200 sweeps, with $+$'s and $\times$'s for the cooling and heating runs. The value of the Gaussian width σ is 0.004 for the U(1) gauge theory calculations. As in the $Z(2)$ calculation, the Gaussian distribution reproduces the equilibrium state far from the transition region, follows the metastable supercooled or superheated states near the transition, and crosses over from one to the other along a smooth s-shaped curve without any appreciable difference between cooling and heating runs. There is some hysteresis visible in the Gaussian results, but it is small compared to the region of the transition, so the equal-area construction of the transition parameters is quite accurate. In practice we average the two results for a given value of S_0 from the cooling and heating runs before making the equal-area construction.

Figure 6 shows the Gaussian results for $\phi=10°$ to 40°, here plotted in the form of β vs $\bar{S}$, appropriate to making the equal-area construction as in Fig. 2. The points plotted as dots and crosses are for cooling and heating runs, respectively, and the curves are the averages of the two points with the same value of S_0 from the cooling and heating runs. This figure shows how the latent heat of the first-order transition along the line BC in Fig. 1 decreases as ϕ decreases toward 0°. Figure 7 shows the Gaussian results for $\phi=60°$ and 70°; here for clarity only the averages

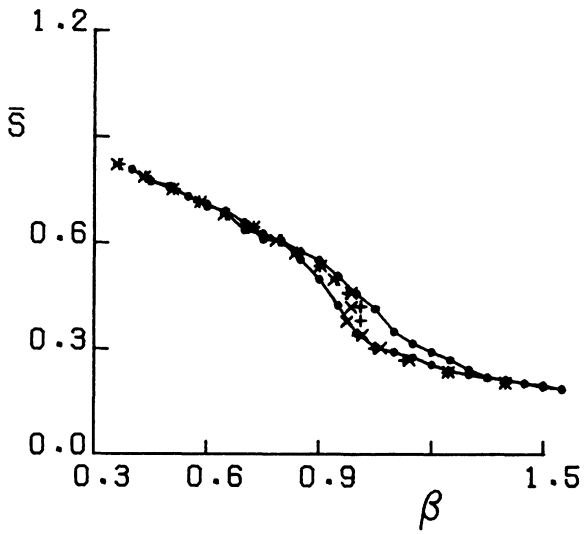

FIG. 4. Average action *per plaquette* $\bar{S}$ vs β for the U(1) gauge theory with $\phi=0°$. The points and crosses have the same meaning as in Fig. 3.

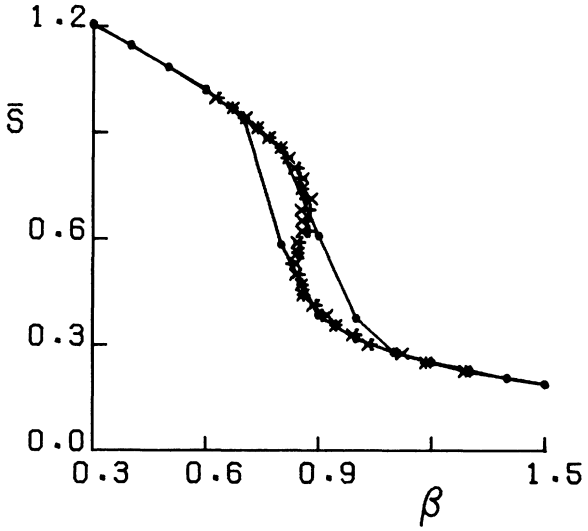

FIG. 5. Average action *per plaquette* $\bar{S}$ vs β for the U(1) gauge theory with $\phi=30°$. The points and crosses have the same meaning as in Fig. 3.

of the points for cooling and heating runs are shown. Figure 7 shows how the strong first-order transition along BC separates into two transitions at B in Fig. 1. For $\phi=60°$ the system has a first-order transition with a large latent heat. For $\phi=70°$ the system has a first-order transition with a much smaller latent heat on the line extending from B toward increasing β_2, and a second-order transition on the line AB; the Gaussian method distinguishes very obviously between the first-order transitions, which show an s-shaped crossover from one phase to the other, and the second-order transition which shows a flat crossover.

The first-order transition points marked on the phase diagram in Fig. 1 were measured from equal-area constructions on the β-vs-$\bar{S}$ curves for different values of ϕ. Figure 8 shows the average action *per plaquette* S_a and S_b at the end points a and b of the s-shaped curve; the difference between S_b and S_a is the latent heat of the transition. The values of S_a and S_b for $\phi=20°$ through 70° are from the calculations described earlier, with 200 sweeps for each value of S_0. For $\phi=10°$ a more lengthy calculation is necessary because the transition becomes weak as ϕ approaches 0; for $\phi=10°$ the Gaussian method was used with 400 sweeps for each value of S_0.

Figure 9 shows the results of calculations using the Gaussian method for $\phi=0°$. The points plotted as dots and crosses show β vs $\bar{S}$ from heating and cooling runs, respectively. Each point is the average of the last 600 of 800 sweeps. The Gaussian width parameter σ is 0.010 in this calculation. The value $\sigma=0.010$ is used rather than 0.004 as in the other calculations, because we find that for $\phi=0°$ the broader Gaussian has less trouble with hysteresis. The error bars on the value of β show the standard deviation assuming the 600 sweeps yield 60 independent measurements, i.e., a correlation length of 10 sweeps; however, since the fluctuations in the transition region are large compared to this standard deviation the correlation length is in fact larger than 10 sweeps. Therefore we also carried out runs of 5000 sweeps for 4 values of S_0; these

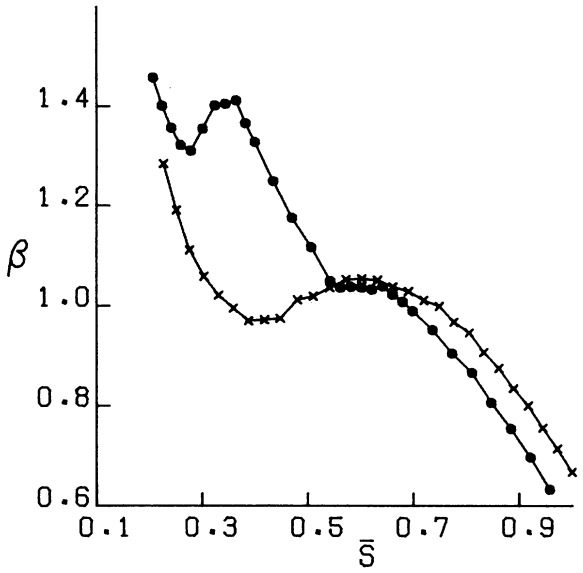

FIG. 7. The β vs $\bar{S}$ curves computed by the Gaussian method for the U(1) gauge theory for $\phi=60°$ and 70°. The crosses and dots are for $\phi=60°$ and 70°, respectively; these are averages of cooling and heating runs.

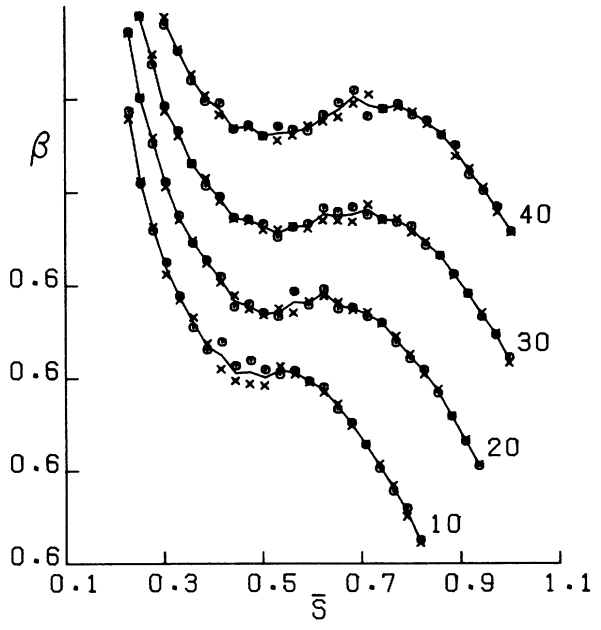

FIG. 6. The β vs $\bar{S}$ curves computed by the Gaussian method for the U(1) gauge theory for $\phi=10°$, 20°, 30°, 40°. The tic marks on the β axis are separated by 0.15 in β. To separate the four curves, $\phi=20°$ is shifted up by one tic mark relative to $\phi=10°$, $\phi=30°$ by two tic marks, etc.; that is, the lowest tic marked 0.6 is for $\phi=10°$, the next one up is for $\phi=20°$, etc. The dots and crosses are from cooling and heating runs, respectively, and the line segments connect the averages of the cooling and heating runs.

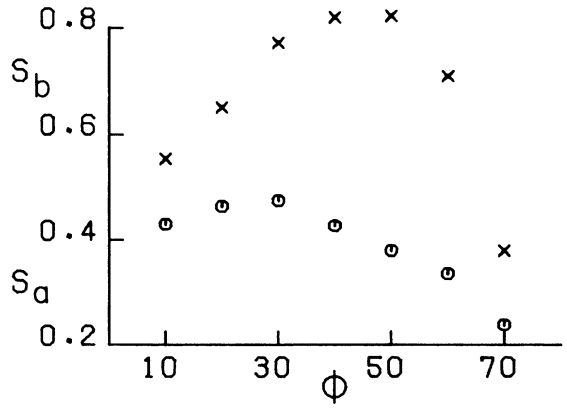

FIG. 8. Action *per plaquette* S_a and S_b at the end points a and b of the transition of the U(1) gauge theory, as a function of the coupling parameter ϕ in degrees. The latent heat is S_b-S_a.

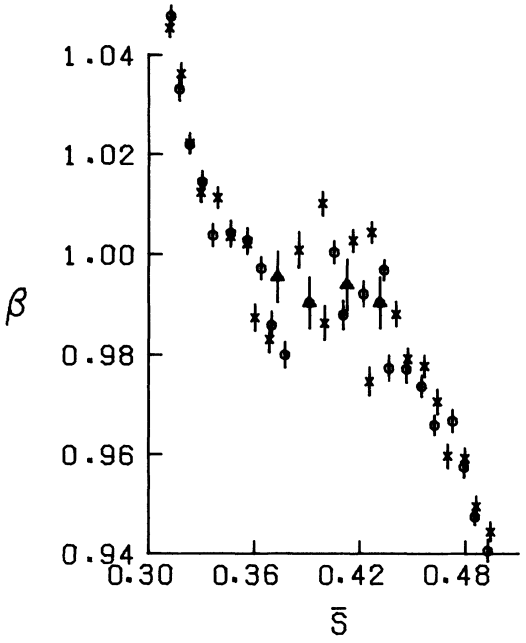

FIG. 9. The β vs $\bar{S}$ points computed by the Gaussian method for the U(1) gauge theory with $\phi=0°$. The points plotted as dots and crosses are for 800 sweeps, heating and cooling runs, respectively; the triangles are for 5000 sweeps. The error bars are explained in the text.

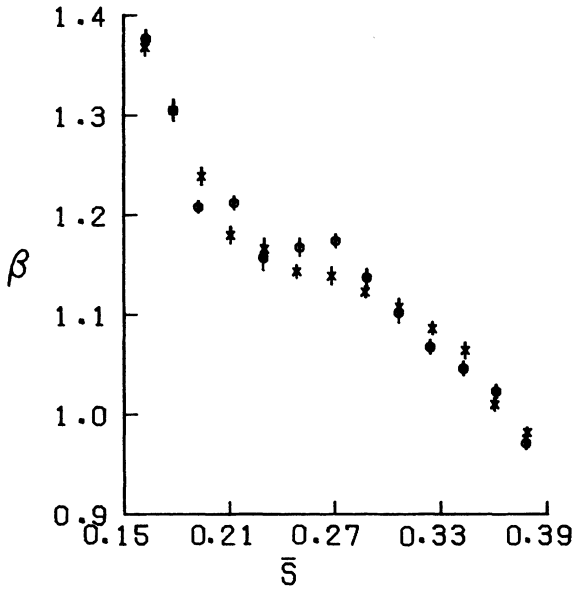

FIG. 10. The β vs $\bar{S}$ points computed by the Gaussian method for the U(1) gauge theory with $\phi=-10°$. The dots and crosses are for cooling and heating runs, respectively.

are plotted as triangles in Fig. 9. For these long runs we accurately determined the uncertainty in β by computing the correlation between different measurements of β in the Metropolis sequence, as a function of the number of sweeps between the measurements. From this autocorrelation function we found that the correlation length is approximately 200 sweeps, so that the 5000 sweeps yield only 25 independent measurements of β; we used this result to obtain the error bars on the triangles in Fig. 9.

Our calculations indicate that for a lattice of size 5^4, the tricritical point occurs very close to $\phi=0°$. This statement is based on three observations. First, for $\phi=0°$ the Gaussian method yields a crossover curve from one phase to the other that is almost flat; there is some hint of an s-shaped crossover, but it is not large enough to be statistically significant within the uncertainty of our results. Second, extrapolation of S_a and S_b from $\phi \geq 10°$ indicates that S_a and S_b are nearly equal at $\phi=0°$. Third, the large Monte Carlo correlation length at the transition temperature for $\phi=0°$ may be a critical slowing down effect associated with the nearby tricritical point.

For $\phi<0°$ the transition becomes smooth. Figure 10 shows the results of a calculation for $\phi=-10°$, with Gaussian width $\sigma=0.004$ and 200 sweeps for each value of S_0. The error bars show the standard deviations using a Monte Carlo correlation length of 10 sweeps. There is clearly a transition at $\beta \simeq 1.15$, but since the curve does not have an s-shaped crossover region we conclude that this is a second-order transition.

IV. SUMMARY

We have described the application of a new Monte Carlo method to study the phase transitions of the $Z(2)$ and U(1) lattice gauge theories. In the new method a Gaussian energy distribution is sampled, rather than the Boltzmann distribution, to describe an equilibrium state of the system. The two parameters of the Gaussian function are a central value E_0 and width σ. The internal energy $\bar{E}$ and temperature β of the system are computed quantities, which are changed by varying E_0. We have not yet studied in detail the dependence of the results on σ. The theory behind this method, based on macroscopic statistical thermodynamics, indicates that the equilibrium state created by sampling the Gaussian distribution is the same as that which would be created by sampling the Boltzmann distribution at the same β, for a large system.

Our results show that this approach to the measurement of the phase transition can be very useful. Effects of hysteresis, while they may not be eliminated entirely, are definitely much smaller than for the conventional approach. The hysteresis may be completely negligible, even for a strong first-order transition, as in the example of the $Z(2)$ gauge theory. Therefore a relatively inexpensive computation is sufficient to obtain an accurate measurement of parameters of the transition.

The calculations on the U(1) lattice gauge theory with mixed charge-1 and charge-2 interactions demonstrate the power of the new approach. The first-order transition along the line BC in Fig. 1 is accurately measured by this method until the transition approaches the tricritical point near C. More extensive calculations, with greater statistical accuracy, for larger lattices, and including a treatment of finite-size effects, may provide an accurate determina-

tion of the tricritical point of this model. Of course there are many other models to which the Gaussian sampling can be applied. As one example, the XY model in three dimensions, with mixed charge-1 and charge-2 interactions, which has recently been shown[8] to have a tricritical point similar to the U(1) gauge theory in four dimensions, could be studied by this method. In the field of lattice gauge theory, interesting models to which this method could be applied are the SU(2) gauge theory with mixed fundamental and adjoint representation couplings,[9] and a lattice field theory that interpolates between U(1) and SU(2) gauge theories.[10]

ACKNOWLEDGMENTS

We wish to thank Murty Challa for several useful conversations. This research was supported in part by the National Science Foundation under Grant No. PHY-83-05722.

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[6]The notation in Sec. II, which is independent of the remainder of the paper, is the notation of traditional statistical thermodynamics. The symbol E (for energy) here corresponds to the symbol S (for action) in the other sections while S in Sec. II refers to entropy.

[7]In the original paper by Metropolis *et al.* (Ref. 1) only the Boltzmann sampling function $\exp(-\beta E)$ seems to be treated. However, for many physicists the "Metropolis method" implies only the more general procedure which can be applied to any distribution. We use this more general definition which has nothing to do with the Boltzmann function.

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