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Monte Carlo study of Abelian lattice gauge theories

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Using Monte Carlo techniques, we study the thermodynamics of four-dimensional Euclidean lattice gauge theories, with gauge groups Z_N and U(1). For $N \leq 4$ the models exhibit a single first-order phase transition, while for $N \geq 5$ we observe two transitions of higher order. As N increases, one of these transitions moves toward zero temperature, whereas the other remains at finite temperature and survives in the U(1) limit. The behavior of the Wilson loop factor is also analyzed for the Z_2 and Z_6 models.

I. INTRODUCTION

Lattice gauge theories currently provide one of the most promising approaches toward a demonstration of quark confinement through an interaction with non-Abelian gauge fields.[1] The lattice formulation introduces a nonperturbative ultraviolet cutoff rendering the theory well defined. Wilson's expansion in terms of strings shows confinement for strong coupling[1]; however, ordinary perturbation theory via a spin-wave expansion suggests a possible unconfined phase for weak coupling. According to conventional lore,[2] four space-time dimensions represent a critical case where the spin-wave phase never appears for non-Abelian continuous gauge groups, but does appear for the Abelian group U(1) describing conventional electrodynamics. This parallels the critical nature of two dimensions for systems of spins interacting through nearest-neighbor couplings; the Heisenberg model based on the non-Abelian symmetry O(3) has only a disordered phase in two dimensions,[3] whereas with the Abelian group U(1) there is also a low-temperature phase with correlation functions behaving as a power of separation at large distances.[4]

Balian, Drouffe, and Itzykson suggested the study of discrete gauge groups as a practice ground for understanding the phase structure of lattice gauge theories.[5] Particularly interesting is the group Z_N, the set of complex Nth roots of unity with ordinary multiplication as the group operation. For $N=2$ we have a gauge-invariant generalization of the Ising model,[6] while when N goes to infinity we obtain U(1), the group of relevance to electrodynamics. In an earlier paper we used Monte Carlo techniques to argue that the Z_2 model has a first-order phase transition at the temperature where the system is self-dual.[7] In this article we extend our investigation to the groups Z_N and U(1).

Our results give evidence for a single, first-order phase transition in the Z_3 and Z_4 theories, at the self-dual temperatures.[8] For larger values of N, the Z_N model appears instead to undergo two phase transitions of higher order, at two temperatures, the higher of which shows little N dependence, whereas the other decreases for increasing N as $[1-\cos(2\pi/N)]=O(1/N^2)$. The former transition survives the U(1) limit. This pattern of phase transitions agrees nicely with recent theoretical arguments that for N large enough the Z_N theory should possess three phases, a disordered one at high temperature, an ordered one similar to that seen in the Z_2 model at low temperature, and a third intermediate phase mimicking the unconfined phase of the U(1) theory.[9] For the Z_6 model, where the two transitions are separated enough to delineate a clear intermediate phase and yet the ordered phase extends to a temperature sufficiently high to allow for an efficient Monte Carlo procedure, we have also studied the behavior of Wilson loops.[1] They appear to decrease exponentially with the area of the enclosed region in the disordered phase and with the perimeter in the intermediate- and low-temperature phases.

In Sec. II we define the models under consideration. Section III reviews the Monte Carlo technique used to evaluate the statistical sums. Section IV presents our results and Sec. V contains a few closing remarks.

II. THE MODELS

We formulate the theory on a four-dimensional hypercubical lattice. Associated with each link joining a pair of nearest-neighbor sites i and j is an element U_{ij} of the group Z_N defined by

$$Z_N=\{e^{2\pi in/N}\,|\,n=0,1,\ldots,N-1\}. \tag{2.1}$$

This set forms an Abelian group under ordinary multiplication. As N goes to infinity we obtain the group U(1). The U_{ij} are oriented on the links of the lattice in the sense that we require

$$U_{ji}=U_{ij}^{*}. \tag{2.2}$$

The action describing the interaction of these

spins is

$$S=\tfrac{1}{8}\sum_{i,j,k,l} P_{ijkl}(1-U_{ij}U_{jk}U_{kl}U_{li})\,, \tag{2.3}$$

where

$$P_{ijkl}=\begin{cases} 1 \text{ if } i,j,k,l \text{ label vertices circulating around an elementary square or "plaquette" of the lattice}\,, \\ 0 \text{ otherwise.}\end{cases} \tag{2.4}$$

The factor of $\frac{1}{8}$ in Eq. (2.3) is inserted because each plaquette is counted eight times in the sum, four times in each of the two orientations. The action is real because the contribution from a definite orientation of a plaquette is the complex conjugate of that for the opposite one. The total contribution from any plaquette to S lies in the interval [0, 2].

We insert this action into a path integral to define a partition function at temperature $T=1/\beta$,

$$Z=\sum_{\{U_{ij}\}} e^{-\beta S}\,, \tag{2.5}$$

where the sum runs over all possible values of the link variables U_{ij}. The "free energy" of the system is an intensive quantity defined by

$$F=\frac{1}{N_s}\ln Z\,, \tag{2.6}$$

where N_s is the number of sites on the lattice. A phase transition is defined as a singularity in the infinite-volume limit of F considered as a function of β. Differentiating the free energy gives the average action per plaquette

$$E\equiv\langle 1-\mathrm{Re}U_{ij}U_{jk}U_{kl}U_{li}\rangle=-\frac{1}{6}\frac{\partial}{\partial\beta}F\,, \tag{2.7}$$

where the sites i, j, k, and l circulate around an elementary square. The factor $\frac{1}{6}$ is the ratio of the number of sites to the number of plaquettes in a four-dimensional lattice. This quantity E is the order parameter we concentrate upon in our numerical work. At a first-order phase transition E is discontinuous in β, while for higher-order transitions it is continuous.

III. THE MONTE CARLO TECHNIQUE

The partition function represents a sum over all configurations of the system, i.e., over all possible values for the statistical variables U_{ij}. Although for a bounded system this is a finite sum, the number of terms involved is so large even for systems of rather small size that it cannot be evaluated directly by numerical methods. In a Monte Carlo computation one generates a sequence of configurations which simulates an ensemble of states in thermal equilibrium at inverse temperature β. A sum over the states in this sequence approximates the full statistical sum.[10]

More specifically, the Monte Carlo technique consists of setting up a Markovian process. At each step a state of the system Σ_i is transformed into a new state Σ_{i+1} (which may coincide with Σ_i) according to a probability matrix $P(\Sigma_i,\Sigma_{i+1})$. This matrix must have the Boltzmann distribution as an eigenvector, i.e., the Markovian process must transform an ensemble in equilibrium into itself. A sufficient condition for this is an equation of detailed balance

$$\frac{P(\Sigma,\Sigma')}{P(\Sigma',\Sigma)}=\exp\{-\beta[S(\Sigma')-S(\Sigma)]\}\,, \tag{3.1}$$

where $S(\Sigma)$ represents the action of the state Σ.

This is quite general and does not determine the probability matrix uniquely. Considerations of efficiency and computational feasibility eventually dictate its form. In our work we have followed the rather common procedure of probing the spins of the lattice one at a time, so that Σ_i and Σ_{i+1} differ at most in the value of a single statistical variable U_{ij}. Properly speaking, then, we are not dealing with a single probability matrix, but rather a collection of matrices $P^{(ij)}(\Sigma,\Sigma')$, one for each statistical variable. The entries of $P^{(ij)}(\Sigma,\Sigma')$ are zero unless Σ and Σ' differ at most in the value of U_{ij}. A single Monte Carlo step consists in acting with one of the $P^{(ij)}$ on the state vector. All the statistical variables are probed in succession, and therefore the matrix defining the Markovian process is

$$P=P^{(i_Nj_N)}\cdots P^{(i_2j_2)}P^{(i_1j_1)}\,, \tag{3.2}$$

where the product runs over all links in the lattice. We shall refer to the application of P to the state vector as one Monte Carlo iteration, or a sweep of the lattice. In other words, the spins are probed in orderly succession and stochastically set to new values. When all the spins have been analyzed, one proceeds to a new iteration.

This still leaves open the detailed form of $P^{(ij)}(\Sigma,\Sigma')$. We have performed computations with two distinct probability matrices, corresponding to different algorithms for the stochastic changing of spins. One method, introduced by Metropolis *et al.*,[11] begins by choosing randomly a new value $U'_{ij}\neq U_{ij}$ from the group elements with uniform probability. If the action is lowered by the replacement of U_{ij} with U'_{ij}, the spin is set to this new value; if $\Delta S\geq 0$, a random number r with uniform distribution between 0 and 1 is generated and the spin is changed to U'_{ij} only if $r<\exp(-\beta\Delta S)$. This simple algorithm ensures that Eq. (3.1) is satisfied.

We have used this method in conjunction with a

computational technique allowing the storage of many spin variables in a single memory word of a computer and involving many spins in parallel computations with logic operations. This procedure makes the actual computations very fast, effectively reducing the dimensionality of the lattice from four to three. We have briefly described this technique in a previous communication[7] and shall not elaborate on it further here. With this method we work on a periodic lattice of 8 sites in the x, y, and z directions, and 20 sites in the t direction. The total number of spin variables is thus 40 960.[12]

As an alternative procedure, we have used an algorithm which selects a new value U'_{ij} for the spin variable in a stochastic manner with probability distribution proportional to the Boltzmann factor $\exp(-\beta S)$. The previous value of U_{ij} plays no direct role in the selection procedure. This method corresponds to placing successively each spin of the lattice in contact with a heat bath and will be referred to by this name. The corresponding probability matrix also obeys Eq. (3.1). The heat-bath method lends itself less well to the multiple storage of spins and the computations involved are slower; however, this is often offset by a faster convergence to equilibrium. In what follows, we shall explicitly indicate those results obtained with the heat-bath technique, leaving it understood that the others were derived by the procedure of Metropolis *et al.*[11] Frequently we have used the two methods independently to evaluate similar quantities as a check on the consistency of the results.

IV. RESULTS

A thermal cycle of a statistical system can provide a general overview of its phase structure. The temperature T is gradually varied while the internal energy is measured. By making the variation of the temperature sufficiently slow, the system can be kept generally close to thermal equilibrium, even though this is in principle never quite reached. In the neighborhood of a phase transition, however, the relaxation time increases and so does the departure from equilibrium. A hysteresis effect will then signal the presence of the transition.

These features, which would be observed in a true experiment, are also apparent in a Monte Carlo simulation. We have therefore evaluated the behavior of E in such a thermal cycle with gauge groups Z_2, Z_3, Z_4, Z_5, Z_6, and Z_8. The results are displayed in Figs. 1(a)–1(f). Starting with a definite value β_0 for the inverse temperature and with a completely ordered configuration where all U_{ij} are set to the group identity, we have performed Monte Carlo computations while changing β slightly after each iteration. Thus β is reduced to zero (infinite temperature) and then returned to β_0. We have chosen β_0 of 1.2 for Z_2, 2.0 for Z_3, Z_4, and Z_5, 2.5 for Z_6, and 3.5 for Z_8. The total number of iterations in the thermal cycles is 4000 for the models Z_2–Z_5, 5000 for Z_6, and 7000 for Z_8. The points are plotted every 16 iterations for Z_2 and every 10 for the other systems.

Hysteresis effects are apparent in all the dia-

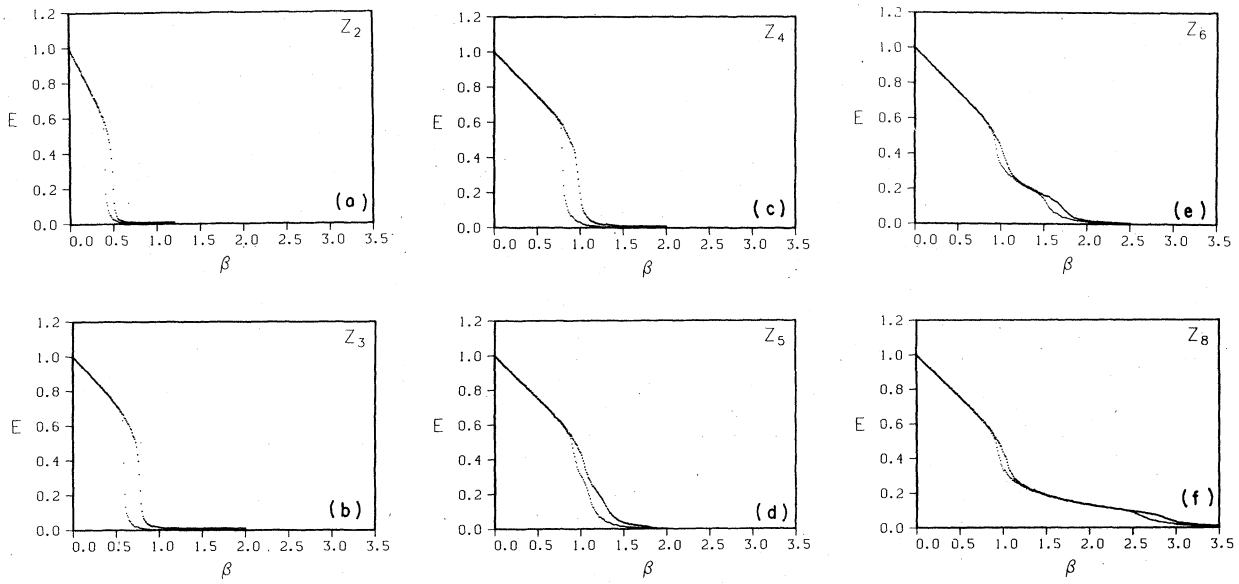

FIG. 1. Thermal cycles on the models Z_2, Z_3, Z_4, Z_5, Z_6, and Z_8.

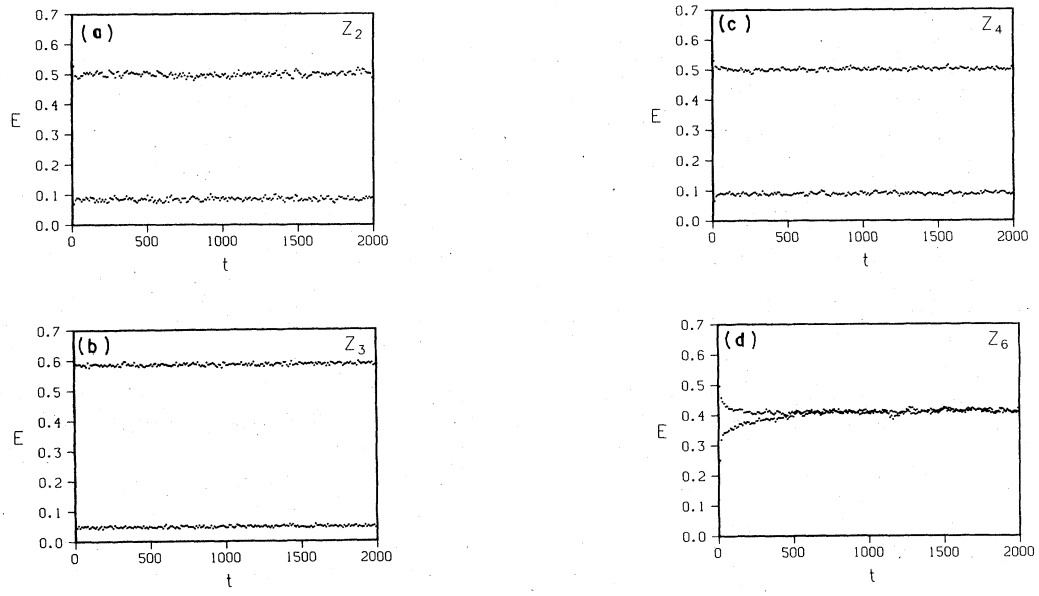

FIG. 2. Long runs at a critical temperature for the models Z_2, Z_2, Z_4, and Z_6.

grams; however, their qualitative features change drastically in the passage from Z_4 to higher groups. For Z_2, Z_3, and Z_4 one observes a single, rather steep hysteresis cycle. With Z_5 the cycle begins to separate into two less steep loops. This doubling becomes manifest with Z_6 and Z_8. Thus, the thermal cycles suggest a single transition with Z_2, Z_3, and Z_4, and two separate ones with Z_6, Z_8, and, most likely, Z_5.

The pronounced jumps in the cycles with Z_2, Z_3, and Z_4 suggest first-order transitions. At the temperature of a first-order phase change, a system can exist in either or two distinct stable phases, an ordered one with smaller internal energy and a disordered one with greater internal energy. Both phases become metastable on the "wrong" side of the transition. At a temperature slightly higher, for instance, than the critical value, the ordered phase is metastable and can exhibit an extremely long relaxation time to equilibrium. This property of superheating or supercooling, which represents a hindrance to reaching equilibrium from an inappropriate starting phase, can be exploited to verify the nature of the transition. Figures 2(a)–2(d) illustrate the results of long (2000 iterations) Monte Carlo simulations with β fixed near a critical point. The values selected for β are 0.4407, 0.67, 0.88, and 1.0 for the models Z_2, Z_3, Z_4, and Z_6, respectively. The critical values $\beta_c = \frac{1}{2}\ln(1+\sqrt{2})$ for Z_2, $\frac{2}{3}\ln[2/(\sqrt{3}-1)]$ for Z_3, and $\ln(1+\sqrt{2})$ for Z_4 are known from the self-duality of these models.[5,8] The value 1.0 for Z_6 was selected on the basis of further analysis presented below. The two series of points in each of these figures correspond to the values of E observed every 10 iterations. The starting configuration was completely ordered for the lower set of points and totally random for the upper set. For the groups Z_2, Z_3, and Z_4 the systems appear to converge in remarkably few iterations to one of the two definite phases, both of which then remain stable. The behavior of the Z_6 model is drastically different; irrespective of the initial configuration the internal energy converges rather slowly to a unique value. This is indicative of a phase transition of higher than first order.

The fact that Monte Carlo simulations starting from a totally ordered and a totally disordered lattice produce internal energies converging to a common value is a good sign that thermal equilibrium is being reached. Unfortunately, in the neighborhood of a first-order phase transition, the convergence of the metastable phase to thermal equilibrium becomes too slow to make this check feasible. To investigate the properties of the system in these regions and to determine the critical value of β more accurately than from a simple inspection of the hysteresis cycles, we have resorted to the following stratagem. A mixed configuration, in which all the U_{ij} with time coordinate between 1 and 10 are set equal to the identity and the remaining half are chosen randomly, has been used as initial configuration. 400 Monte Carlo iterations have then been performed for a few values of β selected in the regions of the hysteresis cycles. The results are displayed in Figs. 3(a)–3(d) for the groups Z_2, Z_3, Z_4, and Z_6. All diagrams show the results obtained with 7

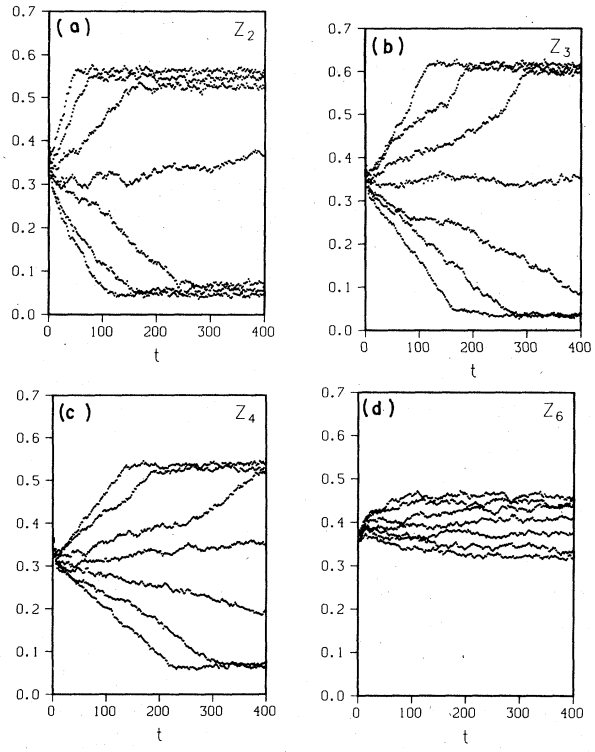

FIG. 3. Mixed phase running with groups Z_2, Z_3, Z_4, and Z_6.

values of β, in steps of 0.01, starting from 0.41, 0.64, 0.85, and 0.97 for the groups Z_2, Z_3, Z_4, and Z_6, respectively, the lower series of points corresponding to larger values of β. For Z_2, Z_3, and Z_4 one notices a quick initial relaxation of the value of E, corresponding to a rapid approach of the two halves of the system to the two phases which can coexist at the critical point, followed by a rather linear drift as the boundary between the two phases shifts until the stable phase overtakes the whole lattice. At the critical temperature both phases are stable and the drift is absent. From Figs. 3(a)–3(c) one can read off the self-dual points $\beta = 0.44$, 0.67, and 0.88 for the models Z_2, Z_3, and Z_4, respectively. The behavior of the mixed phase for Z_6 is strikingly different. One notices a convergence to an equilibrium value of E varying smoothly with β, suggesting a continous transition.

The model Z_6 represents the first case where the three-phase structure is well separated. We have tried to determine E as a function of β in more detail by a series of Monte Carlo simulations where the initial configuration consisted of layers of ordered and disordered spins. Then 500 iterations were performed for values of β set equal to 0.5, 0.9, 0.95, 0.98, 1, 1.02, 1.05, 1.1, 1.3, 1.5, 1.55, 1.58, 1.6, 1.62, 1.65, 1.7, and 2. For $\beta \leq 1.55$ the system appeared to converge to thermal equilibrium; for $\beta > 1.55$ the energy was still moving downward at the end of the 500 sweeps of the lattice; so, in this region we have proceeded for 500 more iterations. The results are represented by open circles in Fig. 4. The other points in this figure are taken from the thermal cycle. Note two regions where the curve $E(\beta)$ becomes steeper. One is clearly outlined at $\beta \approx 1$. In the second region, at $\beta \approx 1.6$, the actual behavior of the curve is confused by rather large fluctuations.

As can be derived by differentiating Eq. (2.7), the mean square fluctuation of E measured in an equilibrium ensemble is equal to $-(1/N_\square)(\partial E/\partial\beta)$ where $N_\square$ is the number of plaquettes in the lattice. The fluctuations are thus related to the specific heat and should increase at a critical point. An analysis of the mean square deviation of E in the region around $\beta = 1$ has produced the results summarized in the following table:

β	$\langle E\rangle$	$N_\square \times (\langle E^2\rangle - \langle E\rangle^2)$
0.9	0.529	0.810
0.95	0.487	0.778
0.98	0.447	0.997
1	0.411	1.28
1.02	0.337	0.586
1.05	0.310	0.441
1.1	0.285	0.560

The increase in $\langle E^2\rangle - \langle E\rangle^2$ at $\beta \approx 1$ is apparent, but the limited statistics does not allow quantitative comparisons.

Diagrams of E versus β have been obtained with the heat-bath method for the Z_{20} and U(1) models [with lattice size of 8^4 for Z_{20} and 5^4 for U(1)] and are reproduced in Figs. 5 and 6. The first phase transition occurs always at $\beta \approx 1$, the second moves to $\beta \approx 16$ in Z_{20} and is not present in the explored range of β in U(1).

For the marginal Z_5 theory, we used the heat-bath method on an 8^4 lattice at $\beta = 1.0$, 1.1, and 1.2. At $\beta = 1.1$ with either a random or an or-

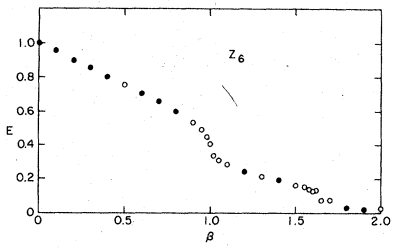

FIG. 4. The internal energy as a function of β for Z_6. The open circles represent the results of the long runs described in the text. The other points are from the thermal cycles.

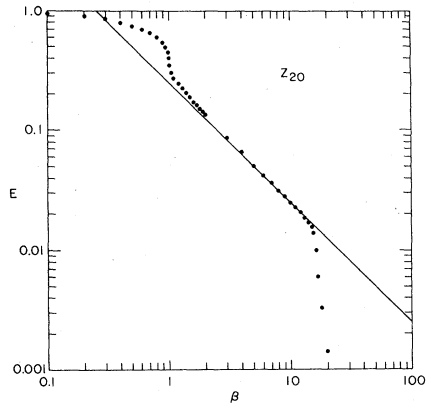

FIG. 5. The internal energy as a function of β for Z_{20}. The straight line represents the asymptotic spin-wave result $1/4\beta$.

dered start the system reached equilibrium within 100 iterations. However, at either $\beta = 1.0$, or $\beta = 1.2$ the convergence rate was substantially reduced and similar to that seen with Z_6 at $\beta = 1.0$. Thus the Z_5 model possesses the three-phase structure of the higher-order groups.

The values obtained for the critical β's are plotted versus the order of the group in Fig. 7. These points are obtained using the heat-bath method and repeatedly adjusting β so that E is maintained in the middle of the hysteresis cycles. The solid line represents the curves $\beta_c = 0.78/[1 - \cos(2\pi/N)]$. The fit suggests that the relevant quantity in determining the position of the low-temperature phase transition is the magnitude of the gap between the action of an unexcited plaquette and the action of a plaquette in its lowest state of excitation.

Finally, we have studied the behavior of the Wilson loop factor, defined as

$$W = \langle \mathrm{Re}(U_{i_1 i_2} U_{i_2 i_3} \cdots U_{i_n i_1}) \rangle , \tag{4.1}$$

where the group elements are associated with links forming a closed loop in the lattice. For an elementary square W equals $1 - E$ and ranges in value between 1, for a totally ordered lattice, and 0, for

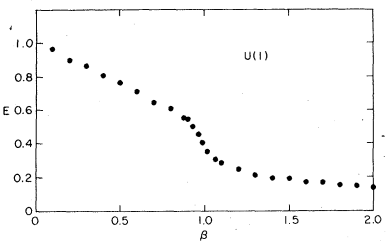

FIG. 6. The internal energy as a function for β for U(1).

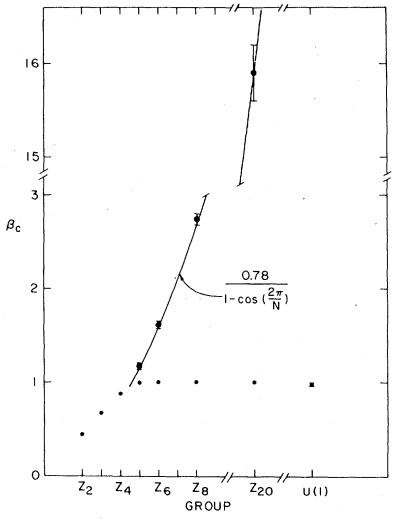

FIG. 7. Critical points as a function of symmetry group.

a totally disordered lattice. If one increases the size of the loop, W always approaches zero (in the limit of ∞ lattice size), but the modality of the approach depends on the phase of the system. It has been argued[1] that in a confining, disordered phase, W decays following an area law

$$W \approx \exp(-cA) , \tag{4.2}$$

A being the area enclosed by the loop, whereas in an ordered, nonconfining phase, W should decay following a perimeter law

$$W \approx \exp(-c'L) , \tag{4.3}$$

L being the length of the perimeter of the loop. In Fig. 8 we compare the values of $1 - W$ for a single plaquette and a square loop of side 2 in the Z_2 model (results obtained with the heat-bath method,

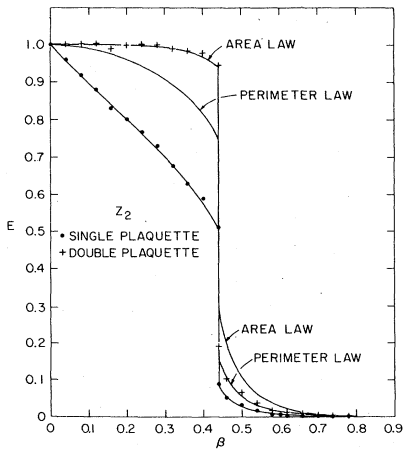

FIG. 8. Square Wilson loops of sides one and two for the group Z_2.

lattice size 8^4). The solid curves represent the predictions of the low- and high-temperature expansions for E and for perimeter- and area-law behaviors of W. The agreement with an area law in the high-temperature phase and with a perimeter law in the low-temperature phase is impressive. In Fig. 9 we plot the quantity $-\ln W$ versus the side of a square loop for a set of values of β in the Z_6 model. In the computations, the loops have been taken spacelike; the periodicity of the lattice then forces $\ln W$ to vanish for a loop of side 8. For the lowest values of β, W rapidly becomes statistically indistinguishable from 0 as one increases the size of the loop and only a few points for $\ln W$ can be plotted. We recall that the phase transition between the high temperature and intermediate phase occurs at $\beta \approx 1$. Correspondingly one notices in Fig. 9 a change from a concave to a rather linear behavior in the curves, suggesting indeed the transition from an area to a perimeter law for W.

V. DISCUSSION

Our work has many features of an experiment. One has a small piece of a four-dimensional crystal, heats it up, cools it, and measures its internal energy. It is, admittedly, a very small crystal, but still one hopes the statistics will be sufficiently good to provide relevant information on the properties of the medium. We have studied the effect of lattice size by performing simulations with the Z_2 gauge theory on hypercubical lattices ranging from 2^4 to 8^4 lattice sites. In Fig. 10 we show the average plaquette and root-mean-square fluctuation at the critical temperature with both ordered and disordered initial conditions. The

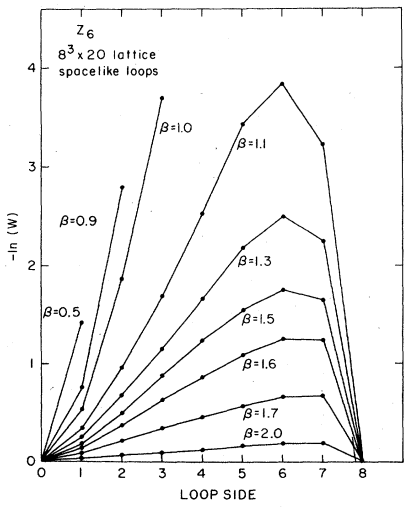

FIG. 9. Square Wilson loops for Z_6 as a function of loop side.

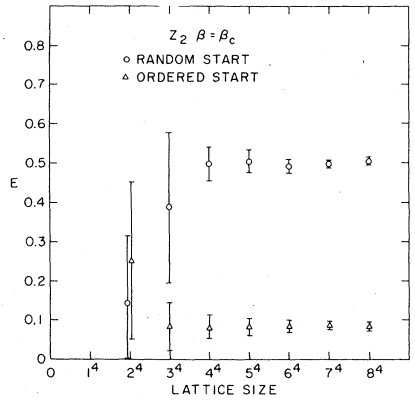

FIG. 10. Size dependence of the two-phase structure with Z_2.

plotted points and error bars are the average over the last 100 of 110 heat-bath iterations. Note that the two-phase structure is already clear on a 4^4 lattice; increasing the size only decreases the fluctuations.

From our work emerges a rather clear phase structure for the abelian lattice gauge theories. The appearance of three phases when the order of the group exceeds 4 is particularly noticeable. It is remarkable that such a structure has been predicted using entirely theoretical arguments based on the approach to the U(1) limit.[9] Our results confirm nicely their analysis.

To a qualitative overview of the thermal properties of the Z_N and U(1) models, we add elements of quantitative information. The curves giving E as a function of β are tantamount to an experimental determination of the partition function. The critical values of β, at which the phase transitions occur, when not known from self-duality, are determined to a reasonable degree of accuracy.

As already noted, the low-temperature transition for the high-order groups scales well with the action of the first excited state above the ground state. For β in the vicinity of this second transition the energy scales approximately as

$$E(\beta) = \frac{1}{\beta} f\left(\frac{\beta}{\beta_2}\right), \tag{5.1}$$

where β_2 is the second critical point and f is independent of the group order. At these low temperatures the large-order models become essentially a gauge-invariant formulation of the surface-roughening model.[13]

Our work supports the existence of a phase transition for U(1) lattice gauge theory. Such a transition is essential if Wilson's formulation is to describe the prototype of all gauge theories, quan-

tum electrodynamics. Indeed, if the approach could not avoid the confinement of electrons, its use for any gauge theory would be suspect. We still have not shown that the low-temperature phase of this system contains a massless excitation, the photon. As some evidence for this, we note that a spin-wave expansion at large β would begin by approximating

$$\mathrm{Re}\left(\prod_{\square} U_{ij}\right) = \cos\left(\sum_{\square}\theta_{ij}\right) \approx 1 - \tfrac{1}{2}\left(\sum_{\square}\theta_{ij}\right)^2 , \quad (5.2)$$

where the group elements are represented as

$$U_{ij} = \exp(i\theta_{ij}) . \quad (5.3)$$

The above replacement makes the path integral Gaussian and solvable, and one finds

$$E \xrightarrow[\beta\to\infty]{} \frac{1}{4\beta} . \quad (5.4)$$

This function is plotted with the results for Z_{20} in Fig. 5. Our results for the U(1) model and the Z_N models in the intermediate phase approach this behavior at large β and thus support the existence of spin-wave excitations.

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