Experiments with a Gauge-Invariant Ising System

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Using Monte Carlo techniques, we evaluate the path integral for the four-dimensional lattice gauge theory with a Z_2 gauge group. The system exhibits a first-order transition. This is contrary to the implications of the approximate Migdal recursion relations but consistant with mean-field-theory arguments. Our "data" agree well with a low-temperature expansion and the exact duality between the high- and low-temperature phases.

Based on a non-Abelian gauge theory, the standard model of hadronic dynamics may simultaneously confine quarks in physical hadrons and possess asymptotic freedom, a vanishing effective coupling at short distances. Central to an understanding of this picture is the study of phase transitions in lattice gauge theory.

Proposed by Wilson as a nonperturbative regularization procedure, lattice gauge theory allows a strong-coupling expansion which demonstrates quark confinement for sufficiently large bare coupling.[1] Nevertheless, conventional weak-coupling perturbation theory suggests a possible electrodynamicslike nonconfining phase. Using mean-field arguments, Balian, Drouffe, and Itzykson have found evidence that in enough space-time dimensions lattice gauge theories will indeed posses two distinct phases depending on the coupling strength.[2] It is essential for the standard model that four space-time dimensions be insufficient for such a transition to occur with an SU(3) gauge group.

Using renormalization-group transformations with approximations based on bond moving, Migdal has argued that four dimensions represent a critical case for lattice gauge theory, just as two dimensions are critical for phase transitions in conventional spin systems with nearest-neighbor interactions.[3] Indeed, Migdal's relations are identical for gauge theory in d dimensions and spin systems in $d/2$ dimensions. Thus, the nonexistence of a phase transition in the O(3) Heisenberg model in two dimensions is touted as evidence for the absence of a nonconfining phase in non-Abelian gauge theories. Further, the interesting and rather complicated phase structure of the X-Y model in two dimensions has been correlated with the possibility of avoiding confinement in a lattice version of electrodynamics based on a U(1) gauge group.

With Wilson's lattice cutoff, one can go beyond the usual continuous Lie groups and consider theories based on discrete groups. The simplest such group is Z_2, the addition of integers modulo 2. As discussed by Balian, Drouffe, and Itzykson, this group provides a gauge-invariant version of the Ising model.[4] The Migdal recursion relation suggests an analogous phase structure between this model in four dimensions and the conventional Ising model in two dimensions. The latter model is exactly solvable and exhibits a second-order phase transition between a disordered and a ferromagnetic state. The purpose of this Letter is to present results, obtained by a Monte Carlo simulation, which strongly indicate that the phase transition in the four-dimensional Z_2 gauge theory is of the first order. Thus, we find evidence of a breakdown of the analogy between this model and the two-dimensional Ising model.

Monte Carlo simulations have provided a useful tool for studying statistical systems of lower dimensionality.[5] In applying this method, one constructs by an iterative procedure a sequence of configurations, Σ_1, Σ_2, Σ_3, ..., which eventually simulates statistical equilibrium. Given any configuration Σ_i, a new configuration Σ_i' is obtained from Σ_i by changing one of the statistical variables (spins) of the lattice. Σ_{i+1} is set equal to Σ_i or to Σ_i' with a definite conditional probability, P, which depends on the actions (or internal energies) of Σ_i and Σ_i'. This probability is chosen so as to ensure that, when equilibrium is reached, the states occur in the sequence with density proportional to the Boltzmann factor. The procedure is continued until all the spins of the lattice have been tested many times and it has become clear that equilibrium has been attained. The states occurring in the sequence then provide a good sample of the correct statistical sum.

A difficulty in the application of the method to four-dimensional systems resides in the large number of spins one has to consider if one wants to incorporate a reasonable number of lattice sites in each linear dimension. To overcome this problem we have developed a technique for processing simultaneously in a high-speed computer all the lattice variables situated along a definite direction, thus effectively reducing a four-dimen-

sional lattice to a three-dimensional lattice of the same linear size. We shall refer to this technique as multispin coding (MSC).

While we shall present details of the technique elsewhere, we mention here the basic underlying idea. MSC takes advantage of the fact that the memory locations, or words, of high-speed computers are designed to store numbers with a high degree of precision, and therefore contain large numbers of binary digits (bits). In a computation where each of the variables can take only the values 0 and 1, representable by a single bit, it is a waste to allocate one word of memory for each spin. By MSC we denote the use of the individual bits of a single memory word to record the values of many different spins. Typically, one may place the spins associated with a fixed value of x, y, z but all values of t in a single word. Besides reducing the amount of memory storage required, MSC allows the simultaneous execution of computations which would otherwise be done sequentially. For instance, suppose that in a Z_2 lattice gauge the bits of the memory words A and B code as ones and zeros the spins located on the links emanating from sites with fixed x, y, z, variable t, and directed along the x and y directions respectively. The "exclusive or" instruction, $C = ([A \text{ and (not } B)] \text{ or } [(\text{not } A) \text{ and } B])$, a simple and fast computer operation, will perform the group multiplication of all the spins in A and B. In other words, MSC turns the computer into a fast array processor.

The Z_2 lattice gauge theory is formulated in terms of spin variables s_{ij} defined over the links of a hypercubical lattice. Each spin $s_{ij} = s_{ji}$ can be 0 or 1; i and j are indices which denote neighboring lattice sites. The action describing the interaction of these spins is

$$S = 2\sum_{\square}\Big(\sum_{s_{ij}\in\square} s_{ij}\Big)_{\mathrm{mod}\,2}, \tag{1}$$

where $\square$ represents a plaquette or elementary square in the lattice, and the outer sum is over all such squares. The factor of 2 is introduced in the definition of S so as to conform with the conventions of Ref. 4.

Working on a lattice of N sites, we define a "free energy"

$$F = N^{-1}\ln Z, \tag{2}$$

where the partition function, Z, is given by

$$Z = \sum_{s_{ij}} e^{-\beta S}. \tag{3}$$

The average action per plaquette is

$$E \equiv (6N)^{-1}\langle S\rangle = -\tfrac{1}{6}dF/d\beta. \tag{4}$$

A phase transition is signaled by a singularity in F or its derivatives. In particular, E should exhibit a discontinuity at a first-order phase transition and should be continuous (but with a discontinuous or singular derivative) at a second-order one.

Some exact results for this model have been obtained. In particular, the model is self-dual,[4,6] the theory at β being related to the theory at $\beta^* = -\frac{1}{2}\ln\tanh\beta$. The self-duality relations for E read

$$E(\beta) = 1 - \tanh\beta - (\sinh 2\beta)^{-1}E(\beta^*). \tag{5}$$

If we assume a unique critical point β_c, self-duality gives

$$\beta_c = \tfrac{1}{2}\ln(1+\sqrt{2}) = 0.4407. \tag{6}$$

We have used a Monte Carlo simulation to calculate $E(\beta)$ for a lattice extending eight sites in the x, y, and z directions and twenty sites in the t direction. To minimize surface effects, we imposed periodic boundary conditions.

We now describe our results. Figure 1 shows the values of E as a function of β obtained in a Monte Carlo simulation where all the spins were probed once and then β was varied slightly before proceeding to another sweep of the lattice. Starting from a completely ordered lattice and $\beta = 1.2$, we reduced β to $\beta = 0$ in steps of 0.0006. At $\beta = 0$ (infinite temperature) the simulation randomizes the lattice. We then increased β back to $\beta = 1.2$

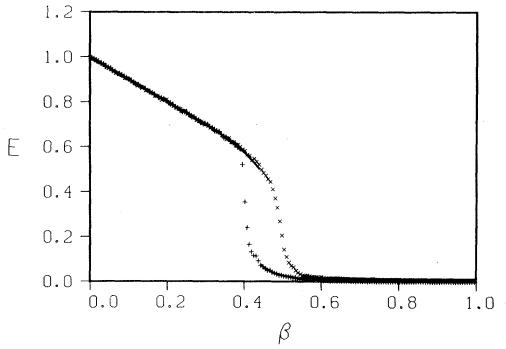

FIG. 1. The average energy per plaquette as a function of β. The system was heated (+) from $\beta = 1.2$ to $\beta = 0$ and then cooled (×) back to $\beta = 1.2$ in steps of 0.0006. Points are plotted every tenth step. The solid curves represent the low- and high-temperature expansions given by Eq. (8) and its dual equation.

with the same step size. In this "experiment" statistical equilibrium is never actually reached; rather, the lattice is heated across the transition temperature first and then cooled back. The clear hysteresis apparent in Fig. 1 is strongly indicative of a first-order phase transition. This hysteresis is due to the metastability of the ordered phase for $\beta<\beta_c$ and of the disordered phase for $\beta>\beta_c$ (superheating and supercooling).

Starting with extreme initial data represented by either a totally disordered configuration (spins chosen randomly) or a completely ordered state (all spins equal to zero), we perform fixed-temperature simulations ranging from a few hundred to several thousand sweeps of the lattice. The length of these simulations was dictated by the time it took the system to reach thermal equilibrium at a given temperature. In Fig. 2(a) we display a typical result of this procedure for $\beta \neq \beta_c$. The graph shows the evolution of the totally ordered state at $\beta=0.425$. After a rapid initial relaxation (on the order of ten sweeps) the system remains metastable for a few hundred sweeps and then abruptly decays into the (high energy) stable phase. In contrast, starting from either extreme initial state, two distinct phases appear to be stable at the critical temperature, with no sign of drift in the value of E, as is shown in Fig. 2(b). This behavior is unique to systems with first-order transitions and, apart from the observed hysteresis, forms the main basis for our conclusions.

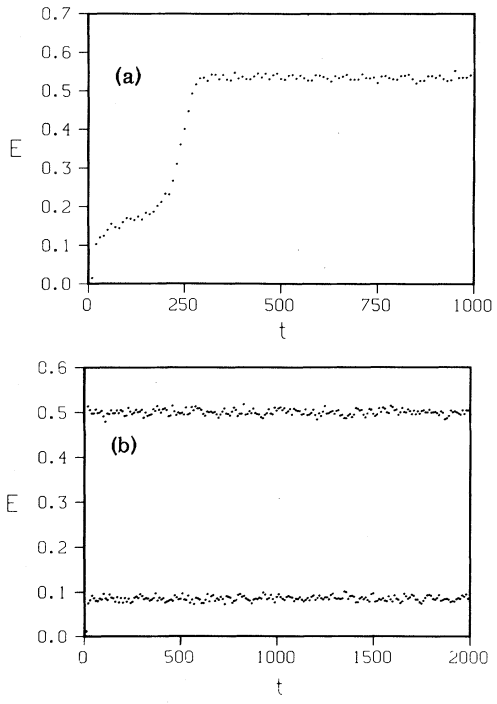

FIG. 2. (a) The evolution of the totally ordered state at $\beta=0.425<\beta_c$. Here t represents the number of sweeps of the lattice. A metastable phase is apparent for $t \lesssim 250$, followed by a transition to the stable phase. (b) The evolution of the totally ordered and the completely disordered states at the critical temperature. One notices the coexistence of two apparently stable phases.

For this system we are fortunate to know the temperature of the transition beforehand. Because of the strong tendency to superheat and supercool, initial conditions entirely in one phase or the other would not permit an accurate determination of an unknown critical temperature. As we wish to study other groups, we need a technique for locating β_c. Therefore we have studied initial conditions with half the lattice randomized and the other half in a ground-state configuration. After a rapid initial relaxation of the two halves into stable or metastable configurations, we observe a linear approach to a single phase. This behavior is shown in Fig. 3. The linear region is suggestive of the unstable phase "dissolving" into the stable phase at the boundary. The direction of this linear behavior determines immediately on which side of the critical temperature one is working.

As a test of our methods, we have carried out simulations on the three-dimensional Z_2 gauge theory. This system is known to undergo a sec-

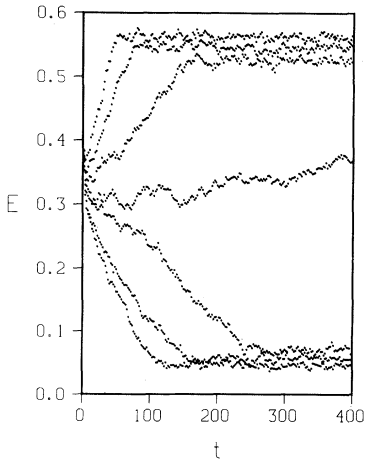

FIG. 3. Plot of average energy vs number of sweeps in the evolution of the mixed phase for (from the lowest curve) $\beta=0.47$, 0.46, 0.45, 0.44, 0.43, 0.42, and 0.41.

ond-order transition at $\beta_c = 0.7613$.[4] The signals alluded to in the preceding paragraphs are absent in this case: given any initial configuration, the approach to equilibrium was gradual; moreover, at β_c both extreme initial configurations evolve smoothly and are seen to merge after a short relaxation time (on the order of 500 sweeps for a $16\times16\times30$ lattice). With use of the mixed phase technique described above, $E(\beta)$ is found to be continuous at β_c, as expected at a second-order transition.

Finally, we wish to remark that a low-temperature expansion can be derived for the system. For the energy we obtain

$$E = 8e^{-12\beta}[1 + 15x^2 + x^3 + 273x^4 + O(x^5)],$$
$$x = e^{-4\beta}. \tag{7}$$

The dual of this expression gives a high-temperature expansion with corrections of order (β^{15}). Equation (7) may be Padé approximated,

$$E = 8e^{-12\beta}\left\{\frac{1 - \frac{1}{15}x - \frac{719}{225}x^2}{1 - \frac{1}{15}x - \frac{4094}{225}x^2} + O(x^5)\right\}. \tag{8}$$

This function and its dual from Eq. (5) are plotted along with the "data" in Fig. 1, with excellent agreement. Note that the expression in Eq. (8) is singular at $\beta \approx 0.36 < \beta_c$. This is presumably an estimate of the maximum temperature for metastability of the superheated phase.

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