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Microcanonical evidence of a first-order phase transition in the four-dimensional U(1) lattice gauge theory

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Using microcanonical Monte Carlo simulations, we present numerical evidence that the phase transition in the four-dimensional compact U(1) lattice gauge theory with the Wilson action is weakly first order. [S1063-651X(96)06211-3]

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The four-dimensional compact U(1) lattice gauge theory is known to have a phase transition that separates a high-temperature confining phase from a low-temperature ''massless'' Coulomb phase [1–3]. The order of the transition is still controversial. Old numerical evidence suggested that this phase transition is second order [4–10]. However, some early simulations and more recent studies [11–14] show a two-state signal at the transition, indicating the possibility of a weakly first-order phase transition, although the evidence presented is numerical in nature and far from conclusive.

The above-mentioned numerical results were obtained using standard canonical distribution Monte Carlo simulations. To study the order of the transition, it may be advantageous to use instead a microcanonical simulation of the system [15–22]. In contrast with canonical ensemble simulations, microcanonical simulations are able to map the metastable and unstable regions of the phase diagram, if they exist, giving a clear signal for the first-order phase transitions. In a microcanonical simulation a characteristic S-shaped curve for the caloric equation of the system $E=E(\beta)$, where E is the internal energy and β the inverse temperature, indicates a first-order phase transition. Evidence of the existence of these metastable and unstable regions for the compact U(1) lattice gauge theory will greatly support the claim of a first-order transition. Failure to see these regions in a microcanonical simulation will be supporting evidence for the claim of a second-order transition.

From the point of view of the microcanonical ensemble, one fixes the internal energy E and computes a microcanonical inverse temperature $\beta=\beta(E)$. A first-order phase transition arises in this context from the existence of a convex region in the microcanonical entropy function $S=S(E)$. This region corresponds to the unstable part of the phase diagram (negative specific heat), and can happen in finite systems. This also suggests that the effect of a first-order phase transition may appear in microcanonical simulations more clearly in small size systems without having to take a formal thermodynamic limit as in the canonical ensemble simulations.

There are several ways of performing microcanonical simulations, all of them more or less equivalent, at least in the thermodynamic limit. For instance, one can introduce an extra degree of freedom, usually called the ''demon'' [14], and let the original system and the demon perform an appropriate random walk with total constant energy E. The demon is allowed to interchange energy with the system, subject to the restriction that its energy cannot be negative. If the system is large enough, the demon will reach thermodynamic equilibrium with a Boltzmann distribution from which one can estimate the inverse temperature β. For a continuous system, and neglecting exponentially small terms, the inverse temperature is obtained by

$$\beta=\frac{1}{\langle E_D\rangle}, \tag{1}$$

where $\langle E_D\rangle$ is the average demon's energy. One can also perform microcanonical simulations based exclusively on the microcanonical distribution [17,18] without requiring a de-

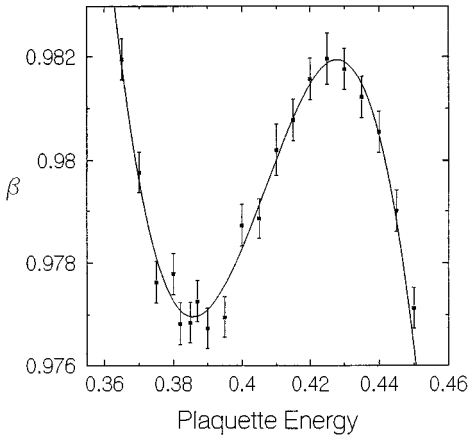

FIG. 1. Results of simulations for lattice linear size $L=4$.

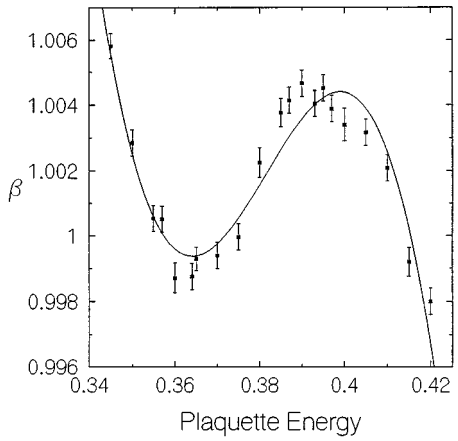

FIG. 2. Results of simulations for lattice linear size $L=6$.

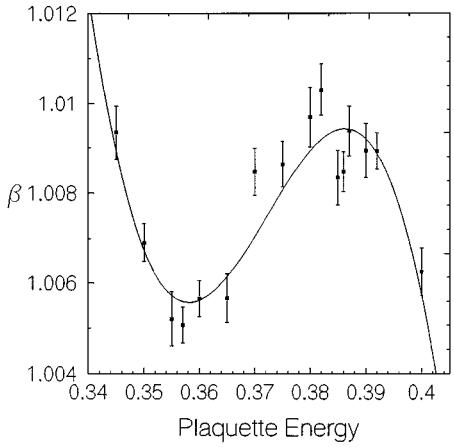

FIG. 3. Results of simulations for lattice linear size $L=8$.

mon that reaches thermodynamic equilibrium. If $\Gamma(E)$ is the volume of phase space with energy less than or equal to E, the microcanonical ensemble entropy $S(E)$ can be defined by

$$S(E)=k_B \log_e(\Gamma(E)), \tag{2}$$

where k_B is the Boltzmann constant. In the absence of a first-order phase transition, $S(E)$ is concave everywhere. The inverse temperature β is computed from Eq. (2) by

$$\beta=\frac{1}{k_B T}=\frac{1}{k_B}\frac{\partial S(E)}{\partial E}=\frac{\partial \log_e(\Gamma(E))}{\partial E}. \tag{3}$$

To test for the presence of a convex region in $S=S(E)$, we only need to evaluate numerically the last derivative in Eq. (3), and look for regions in which β increases with E (unstable region). To achieve this we can approximate numerically this derivative [17]. If ΔE is a small energy increment, we can obtain β numerically by

$$\beta\approx\frac{\log_e(\Gamma(E)/\Gamma(E-\Delta E))}{\Delta E}. \tag{4}$$

The ratio of phase space volumes inside the logarithm in Eq. (4) can be estimated by counting the number of times that, in an appropriate random walk in phase space, the system visits the region with energy between $E-\Delta E$ and E.

One can compute β using Eq. (4) and (1) simultaneously if one assumes that, as the system moves in the random walk, the demon has energy E minus the energy of the system. This allows us to double check that the assumption of thermal equilibrium for the demon gives the same results as the microcanonical ensemble.

For our simulations we have used a four-dimensional cubic lattice with periodic boundary conditions, and linear sizes L of 4, 6, and 8. For the Hamiltonian of the system we have used the standard Wilson action [23]

$$H=\sum_{\text{Plaq}}(1-\cos(\theta_p)), \tag{5}$$

where θ_p is the angle associated with each plaquette of the lattice, and the sum in Eq. (5) is over all oriented plaquettes. For the purpose of the simulation we have discretized the U(1) group to a Z_{5000} group.

The results of the simulations for the three lattice sizes ($L=4$, 6, and 8) are shown in Figs. 1, 2, and 3. As it is to be expected, the data for the larger lattice ($L=8$) is more noisy. It is, however, accurate enough to see clearly the existence of metastable and unstable regions. The solid lines in the figures are only to guide the eye, and are the cubic polynomial fit to the data near the transition. Each point in the figures was obtained from averages over $5–10\times10^6$ lattice updates. The inverse temperatures computed with Eqs. (1) and (4) were in all cases consistent within the statistical uncertainties of the simulation. There is also an expected small shift of the temperature of the transition as the system converges, for larger lattices, to the thermodynamic limit.

These figures show very clearly a very small (note the scale in the β axis) unstable region, of approximately the same size for the three lattices used, indicating that the transition is of first order. The difference in β from the bottom to the top of the unstable region is only about 0.004–0.005. Note that because of the small size (in beta) of the metastable regions, a large number of Monte Carlo iterations are necessary to resolve it. These results give strong support to the claim that the transition in the pure compact U(1) lattice gauge theory is weakly first order. Simulations involving larger lattice sizes and with coupling to Higgs fields are underway, and will be presented elsewhere [24].

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