Finite-size effects and phase transitions

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(Received 27 April 1987; revised manuscript received 8 February 1988)

We perform numerical simulations of SU(2) lattice gauge theory on $4L^2\ 64$ lattices with $4 \le L \le 16$. A finite-size scaling analysis of the tunneling signal extrapolates the critical coupling β_c (relevant for the deconfining phase transition with $N_t=4$) toward the infinite-volume limit and yields $2.28 < \beta_c < 2.32$. We illustrate the method with exact results for the two-dimensional and numerical results for the three-dimensional Ising model. For finite systems the notion of a "phase transition" is discussed critically. Geometry is important and the deconfining phase transition is not sharp on lattices that are relevant for spectrum calculations.

For obvious reasons, Monte Carlo (MC) simulations[1] [of four-dimensional (4D) pure SU(n) lattice gauge theories] are performed on finite lattices. Here, we use periodic boundary conditions. Mass measurements are best done on (N^3N_z, $N_z \gg N$) lattices. Looking at the correlation function's falloff in the z direction allows one to estimate the spectrum of the Hamiltonian in a N^3 box. For technical reasons[2] N_z should be taken as large as possible, although the spectrum is independent of the value chosen for N_z. Such lattices are called $N^3\infty$ lattices hereafter.

Independently, lattice gauge theories are known to exhibit a finite-temperature phase transition.[3] One considers lattices of size N_tN^3, ($N \gg N_t$), interpreted as systems of volume N^3 at inverse temperature N_t (Ref. 4). In the thermodynamical limit $N \to \infty$, N_t fixed, the system presents two phases, a confined phase for $\beta < \beta_c(N_t)$ and a deconfined phase for $\beta > \beta_c(N_t)$ where the global Z_n symmetry (of pure lattice gauge theories) is broken. (As usual, $\beta = 2n/g^2$, where g^2 is the coupling constant.)

This phase transition is a finite-size effect: namely, N_t is small. A natural question to ask is whether the usual finite-size effects (where more than one direction are small) are related, in some sense, to the deconfining phase transition. It is a widespread belief that this relation is strong and that the $N^3\infty$ lattice is in the "deconfined" phase for $\beta > \beta_c$. [Here $\beta_c(N) = \beta_c(N_t = N)$ as determined from finite-temperature studies on N_tN^3, ($N \to \infty$) systems.] This belief is not based on firm ground. The two geometries are very different and the belief has to cope with the fact that, for fixed N, a N^3N_z lattice does not undergo a phase transition for $N_z \to \infty$. This shows up if one tries to locate a transition and/or crossover by looking at the order parameter (i.e., the mean Polyakov loop in any of the three "short" distances). Even if β is large enough such that order takes place and Polyakov loops tend to be aligned, macroscopic domains will exist, the net effect of those being that for $N_z \to \infty$ the crossover moves toward infinity. For $N_z = \infty$, the average Polyakov loop is zero, configuration by configuration. The reason is that, starting from a completely ordered situation (all loops aligned), the energy cost to create a domain (a z interval, where all loops have been rotated by a Z_n element) is (small and) independent of the domain size. It is $2N^3\mathcal{A}$, where $\mathcal{A}$ is the surface tension. For N_z large, a typical configuration will thus contain many domains. The system does not choose one of the n possible ground states but rather a unique linear combination. Tunneling between would-be-degenerate vacua (domain formation) lifts the degeneracy and restores the Z_n symmetry.

The statement that in a finite system a transition is not sharp seems to be standard terminology. Already the example of the Polyakov loop expectation values shows that, to be precise, one has to distinguish two aspects of this terminology. (a) The sharp transition and/or crossover smoothens out. (b) Its location in β moves. Often the second aspect seems to be regarded as irrelevant, presumably because the effect is considered to be a small correction as compared with the first one. This is not necessarily true. In the case of Polakov loop expectation values the signal moves, with $N_z \to \infty$, all the way to $\beta = \infty$. Because of the strong N_z dependence this example looks somewhat artificial and it is natural to ask for the behavior of signals that are N_z independent. A large class with this property are all signals that can be expressed as functions of eigenvalues of the (N_z direction) transfer matrix. In a numerical lattice calculation one normally estimates such eigenvalues from correlation functions.

Correlation functions of Polykov loops (in the fundamental representation) characterize directly the broken or unbroken phase. Here we consider correlations between two zero-momentum Polyakov loops [closed in the (a) small direct direction] separated by a distance z (in the large direction)

$$C(z)=\langle P(0)P(z)\rangle \sim \exp(-N\kappa z) \quad (z\to\infty) .$$

Here N is the length of the loop and κ the string tension[5] (more precisely the energy of a 't Hooft electric flux per unit length). If the symmetry is broken, Polyakov loops are aligned over the whole lattice, $C(z)$ is thus constant for large z, κ is zero. On finite systems κ will never be zero, the phase transition will appear as a rapid crossover to very small κ values.

Other eigenvalues of the transfer matrix, for example, those related to glueball masses, are also expected to be sensitive to the deconfining phase transition, although they are not directly related to the Z_N symmetry. For instance, in the $N_t\infty^3$ geometry one might expect massless gluons at temperature $T=T_c$. In this paper we do not obtain explicit results for the finite-size behavior of glueball masses. Indirectly, our results suggest that reliable *a priori* expectations on this topic are not possible, at least on the basis of current rather limited theoretical knowledge of the dynamics of non-Abelian gauge theories.

For SU(2) lattice gauge theory, the breaking of the Z_2 symmetry invites Ising-model analogies. The mass gap m of an Ising model corresponds to $N\kappa$ and we like to illustrate our investigation first with the solvable 2D Ising model. Consider a LN_z Ising system

$$Z=\sum_{\sigma_i=\pm 1,\sigma_j=\pm 1} \exp\left[-\beta\sum_{nn}\sigma_i\sigma_j\right] ,$$

$$\beta=\frac{1}{T} \quad (T \text{ temperature}) ,$$

and spin-spin correlations in the z direction. The corresponding mass gap is exactly known[6] for any L (and periodic boundary conditions):

$$m=\epsilon_0+\tfrac{1}{2}\sum_{\nu=0}^{L-1}\epsilon_{(\pi/L)(2\nu+1)}-\tfrac{1}{2}\sum_{\nu=0}^{L-1}\epsilon_{(\pi/L)(2\nu)} ,$$

where ϵ_q is the positive root of $\cosh(\epsilon_q)=\cosh[-2\beta-\ln\tanh(\beta)]+[1-\cos(q)]$ for $q\neq 0$ and $\epsilon_0=-2\beta-\ln\tanh(\beta)$. In the high-temperature region, ϵ_0 is positive. It is equal to the infinite-volume mass gap. As L goes to infinity, the two sums cancel out:

$$m\sim\epsilon_0\left[1+O\left[\frac{1}{\sqrt{L}}e^{-\epsilon_0 L}\right]\right] \quad (L\to\infty) . \tag{1}$$

ϵ_0 changes sign at the critical point $\beta_c=\frac{1}{2}\ln(1+\sqrt{2})$, where

$$m=\frac{c}{L}+O\left[\frac{1}{L^2}\right], \quad L\to\infty . \tag{2}$$

In the low-temperature phase, m is exponentially small,

$$m=O\left[\frac{1}{\sqrt{L}}e^{-|e_0|L}\right] . \tag{3}$$

Figure 1 shows the mass gap m as function of the temperature $1/\beta$ for various values of L. The envelope is the infinite-volume result where m is zero in the whole broken phase.

The following comments are in order.

(i) Symmetry breaking means that several (here two) degenerate ground states are possible. The zero mass gap m is nothing but the gap between these degenerate states [see Eq. (3)].

(ii) The infinite-volume limit is often defined in the presence of a small magnetic field H ($\lim H\to 0^+$, volume$\to\infty$). In such circumstances, the system stays trapped in one vacuum and the mass gap, defined through connected correlation functions, is zero at the critical point only (if the transition is second order, otherwise it is never zero). Without a magnetic field, there is no difference between connected and plain correlation functions, as the subtracted expectation values are zero. [Obviously, they may be different in a Monte Carlo (MC) simulation with finite statistics. Convergence to the true results is fastest, if plain correlation functions are used.]

(iii) The behavior of the mass for large L and β follows from the simple domain-wall picture. A (minimal surface) wall contributes by a factor of $e^{-\mathcal{A}L^{(d-1)}}$ to the partition function of a $L^{d-1}N_z$ Ising system, where $\mathcal{A}=2\beta$ holds for the surface tension at large β. Let us consider the correlation function of two spins separated by a distance z. Configurations with n walls between the two spins contribute by a term

$$\sim(-)^n(e^{-2\beta L^{(d-1)}})^n\frac{z^n}{n!}$$

to the correlation function. Summing over all contributions gives

$$C(z)\sim\exp(-ze^{-2\beta L^{(d-1)}})$$

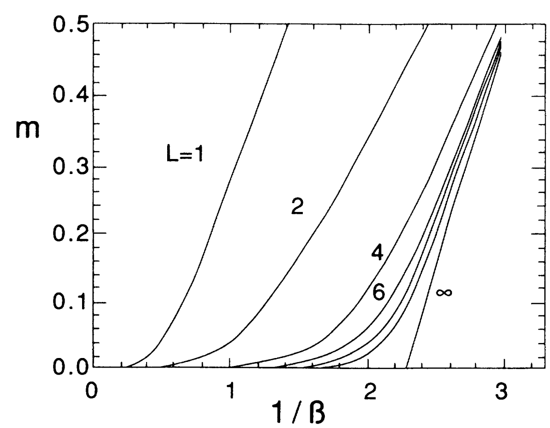

FIG. 1. Mass gap of the 2D Ising model on LN_z lattices. m is plotted vs $1/\beta$ for $L=1$, 2, 4, 6, 8, 10, and infinity.

and therefore

$$m \sim e^{-2\beta L^{(d-1)}} .$$

The correct (power of L in the) prefactor can be obtained by a more careful treatment of the interface.[7]

(iv) The behavior of m for $\beta < \beta_c$ (1) and $\beta > \beta_c$ (3) is quite general. Equation (2), $m \sim 1/L$ (L=large) at $\beta = \beta_c$, is implied by finite-size scaling[8] theory for second-order phase transitions.

The mass-gap behavior (1)–(3) as a function of the lattice size suggests a method to locate the critical point which amounts to plotting $m(L)L$ as function of L for various β. At low β, mL is soaring linearly with L. For larger and larger β the slope will decrease, up to the critical point where mL is constant for large L. Above β_c, mL will decrease with L (faster and faster as β grows).

The method is exemplified in Fig. 2 for 2D and 3D Ising models. mL is plotted as a function for L for $T = T_c$, $T_c(1\pm1\%)$, and $T_c(1\pm5\%)$. The 3D Ising model is of particular interest because spin correlations in this model are in analogy with Polyakov loop correlations in 4D SU(2) lattice gauge theory.[9] Our MC results were obtained running a variant of the computer program of Ref. 10 that uses different random numbers for all 64 lattices. For the critical temperature we assume $T_c = 0.221\,65$ (Ref. 11) and our calculation of zero-momentum correlation functions is carried out on L^2 64 lattices. Evidence is found that the correlations are dominated by a single mass. Therefore, the determination is already possible from effective masses[2] at distances $z=1$ and 2 (the average is used for the figure). In this case our calculation of β_c is, of course, far less accurate than the very precise result of the literature.[11] For SU(2) lattice gauge theory, treated now, the precision turns out to be competitive with previous results.

Before we report the analog MC calculation for SU(2) lattice gauge theory, we would like to comment on finite continuum boxes as used for Lüscher's small-volume calculations.[12,13] The reason is that we[14] first developed concepts, on which this paper relies, when we explored the relationship between the so-called "tunneling transition"[13] and the deconfining phase transition. A continuum box can be defined by taking the limit of lattice gauge theory in a N^3 box, $N \to \infty$, mass gap $m \to 0$ in lattice units, with[8]

$$z_m = Nm = \text{const} .$$

For z_m exactly zero, the Z_n symmetry is broken and the string tension is zero. For any finite z_m, tunneling restores the symmetry and the string tension gets exponentially small contributions like in the Ising-model case (3). The tunneling transition, sharp increase of the string tension as the coupling constant grows, is nothing but a signal for the deconfinement phase transition, maimed by the geometry.[14] Now, we use the tunneling transition to calculate explicitly the critical coupling constant.

Let us consider lattices of size NL^2N_z, $N \le L \le N_z$, N_z very large, and measure correlation functions of two Polyakov loops in the "N direction," separated by a distance z (in the "N_z direction"). For $L=N$, this is just the geometry used for mass-ratio computations.[12,15] Letting L grow enables a true phase transition. For our exploratory demonstration, we have chosen $N=4$ and $N_z=64$, with $4 \le L \le 16$. The analog of $m(L)$ [to which Eqs. (1)–(3) apply] is $N\kappa(L)$ and for various β, $LN\kappa(L)$ is plotted as function of L in Fig. 3.

In the symmetric case[14] ($L=4$), $LN\kappa$ is a rather smooth function of β. The behavior becomes more and more abrupt as L increases. In conclusion, for $\beta \le 2.28$ $LN\kappa$ is clearly increasing with L. On an infinite lattice, this will be the confined region. $\beta \ge 2.32$ will be the deconfined region. Therefore, our estimate is

$$2.28 < \beta_c < 2.32 . \tag{4}$$

This has to be compared with the conventional estimates 2.29±0.01 (Ref. 16) and 2.296±0.005 (Ref. 17). The results are in good agreement. (The small error bars of the standard results involve assuming Ising-model values for certain[16,17] critical exponents.)

More interesting than the number (4) is the behavior

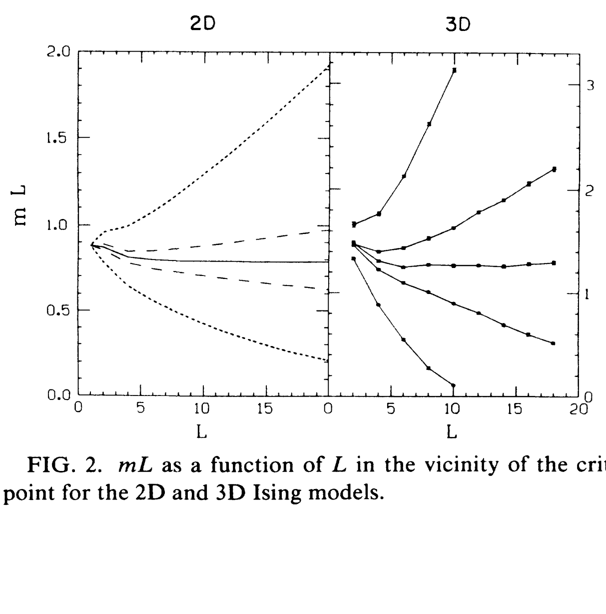

FIG. 2. mL as a function of L in the vicinity of the critical point for the 2D and 3D Ising models.

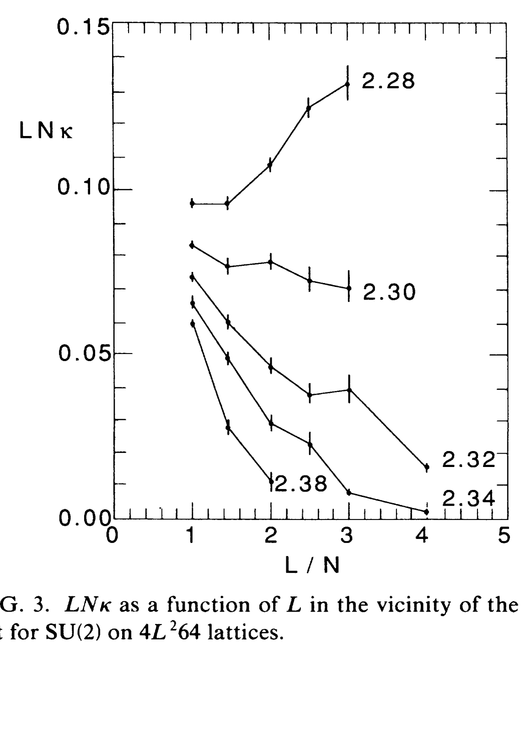

FIG. 3. $LN\kappa$ as a function of L in the vicinity of the critical point for SU(2) on $4L^264$ lattices.

seen in Fig. 1, which is qualitatively also true for $N\kappa$ in lattice gauge theory (N fixed). It implies that on $N^3\infty$ lattices, as relevant for spectrum calculations, the β dependence is smooth around $\beta \approx \beta_c(N_t = 4)$. A remnant of the deconfining phase transition, the tunneling transition, is shifted to a much higher β value [in our SU(2) case $\beta \approx 4.5$, corresponding to $z_m < 1$ (Ref. 2)] The reader should compare the $L = 4$ situation of Fig. 1 which is roughly similar. Let us denote by "intermediate volume" the region between the tunneling transition and $\beta = \beta_c(N)$ on an $N^3\infty$ lattice. By analogy with Fig. 1 we expect that a smooth interpolation of the string tension from the intermediate to the large-volume region exists. Otherwise one would be faced with the strange scenario of two deconfinement remnants in one physical quantity.

For glueballs (in the $N^3\infty$ geometry) the situation is not clarified by results of this investigation. Although the $A1^+$ and E^+ glueball states[15] were also measured (detailed results will be reported elsewhere[2]) and the same smoothness as for the string tension is found around $\beta \approx \beta_c(N_t = 4)$, the situation is nevertheless different. In contrast with the string tension none of the glueballs exhibits a clear deconfinement signal for $\beta > \beta_c(N)$. The present investigation leaves two scenarios open: Either the deconfining transition is entirely smoothened out for glueball states, or remnants of it exist at least for some glueball states and may be shifted to $\beta < \beta_c(N)$. To decide between these two options seems only possible *a posteriori*, i.e., by explicit calculation. Unfortunately our signal-to-noise ratio becomes bad for $\beta < \beta_c$. If the second scenario is realized, the terminology "deconfining phase transition" is rather meaningless on $N^3\infty$ lattices, because equivalent signals for this transition would scatter far beyond their individual accuracy. For finite systems one should only talk about "phase transitions," if relevant signals for it show up *together* in a sufficiently small-β region. The terminology "not sharp" may still be used, but we have to be aware of the fact that it would make rather extreme use of its property (b) stated before. The phase transition has not only become smooth in β due to the finite lattice, but different "smooth" signals may in addition scatter over an even much larger β range.

In conclusion, we have introduced an alternative way of estimating the deconfinment temperature of pure lattice gauge theories. On $N^3\infty$ lattices, as relevant for spectrum calculations, the deconfining phase transition is not sharp (in the sense explained).

Notes added. (1) Since this work was submitted for publication new results, relevant for the $N^3\infty$ case, appeared.[18–20] They suggest other remnants of the deconfining phase transition at $z_m \gg 1$ values. If confirmed, they would decide between the two options that are still left open by the investigation presented here. (2) The method of this paper has turned out to be relevant for the first analytical estimate of the SU(2) deconfinement temperature.[21]

We benefited from discussions with Anna Hasenfratz, Peter Hasenfratz, and Claus Vohwinkel. This research project was partially funded by the Department of Energy under Contracts Nos. DE-FG05-87ER40319 and DE-FC05-85ER25000. It also received support from the Florida State University through use of its CYBER 205.

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