Order of the Deconfining Phase Transition in Pure-Gauge QCD

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We study the behavior of the string tension in the SU(3) lattice pure-gauge theory close to the deconfining critical point. We find very large correlation lengths, increasing with the lattice size. This result is strongly suggestive of a second-order phase transition, and excludes the presence of a strong first-order transition.

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The conjecture that QCD liberates quarks at high temperature, in connection with the existence of a phase transition in a non-Abelian gauge theory, is thirteen years old.[1] Universality arguments have been first advocated in Ref. 2 in order to support a first-order transition. The argument uses the fact that the critical behavior of 4D QCD is described by an effective 3D three-state spin theory. Then universality arguments lead one to argue that the transition has to be first order.

The problem is very specific to SU(3) gauge theory, or better to its center Z_3. In this case one can write a non-symmetry-breaking "φ^3" term in the potential, which according to the Landau criterion would produce a first-order transition. Also the 3D three-state Potts model, which is supposed to support, in such a scenario, all the universality arguments, is a very special case. The problem of the order of the transition of such a model is very contoversial.[3,4] Indeed it is well known that there are transitions which change from first to second order when apparently irrelevant terms are added to the action[3,4] (for example, in the Z_3 model is 2D).

The other main evidence used in order to claim that we are dealing with a first-order transition comes from the early Monte Carlo (MC) simulation work.[5] The recognition of the order of a phase transition is extremely delicate if it is first order, but there is a nearby (in the metastable region) second-order one. In most of the MC simulations done for pure-gauge QCD two different criteria were used to identify a first-order transition: metastabilities near β_c and discontinuities in the thermodynamical quantities. The observation of metastabilities may hardly distinguish between a first-order transition and a second-order one, especially if the quantity that we consider has a behavior like $|T-T_c|^\beta$, with a small β. Indeed also near a second-order transition the equilibration time is divergent and very long relaxation times are present. MC simulations in the 2D Ising model ($\beta=\frac{1}{8}$ for the magnetization) show *clear* signatures of metastability.[6] In principle the observation of discontinuities would be a very clear cut evidence for a first-order transition. Unfortunately discontinuities can never be observed in finite-volume simulations because the transition is rounded. Only a careful (not yet done for QCD) study of the dependence of the rounding with the volume

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can tell us if the rounding is going to disappear in the infinite-volume limit. We firmly believe that the order of a transition can be determined numerically only by using finite-size scaling analysis. Most of the data published up to now can hardly be used to get firm conclusions about the nature of the transition because of the absence of any detailed comparison of results obtained on different finite volumes.

In this Letter we present a very different approach. It consists principally in the measure of the correlation length ξ (i.e., of the string tension σ) close to β_c. For a first-order transition ξ remains finite at β_c, and we expect that ξ is a discontinuous function of the coupling when we go across the transition point. On the other hand, for a second-order transition, $\xi \to \infty$. A similar approach has been followed in Ref. 7, but the improvements in techniques (smearing, source, ...) that we use and the high statistics that we can get are crucial in allowing us to get good quantitative results.

In a finite lattice we have no chance to measure an infinite ξ, and, as in thermodynamical measures, the discontinuity becomes a continuous jump; but now it is possible to relate a finite ξ with finite-lattice effects. If we work in a toroidal space geometry ($L \times L \times L'$ lattice, with $L' \gg L$) ξ cannot exceed L by a large amount, and so the finite-size effects can be monitored by carrying out computations at different lattice sizes. If at β_c we find $\xi \sim L$, this is a clear signature of the fact that ξ is diverging in the thermodynamical limit.

The finite-temperature field theory is defined on an asymmetric periodic lattice of size $L_x \times L_y \times L_z \times L_t$, where $L_t \ll L_x = L_y \ll L_z$. The temperature $T = 1/L_t a$ can then be controlled by changing β, so that the transition temperature will correspond to a given value $\beta = \beta_c$. The Polyakov loop is defined as

$$P(x,y,z) = \tfrac{1}{3} \operatorname{Tr} \prod_{t=1,L_t} U_\tau(x,y,z,t), \tag{1}$$

where U_τ is the link variable in the t direction.

The expectation value of the Polyakov loop is the relevant order parameter; it is zero when $\beta < \beta_c$ and different from zero when $\beta > \beta_c$. A serious problem on a finite lattice is the absence of spontaneous symmetry breaking. Because of tunneling effects the order parameter is always zero. This problem can be circumvented by some *ad hoc* prescriptions; for example, one can take the absolute value of the order parameter before computing the statistical average over configurations. Strictly speaking, this is no longer an order parameter in this case, because such an expectation value is nonzero both above and below T_c. In this context the determination of β_c has a certain level of arbitrariness on a finite lattice.

We decided to use a *source*; i.e., we fix the state of all the x, y, and t link variables at $z = 1$ to the identity. In this way we select, in the phase in which the symmetry is spontaneously broken, a preferred vacuum. The source method not only avoids the tunneling problem, but generates a very strong signal that can be measured at large distances from the source. In fact, we are able to fit an exponential decrease of the Polyakov loop by discarding up to six z slices, and using the data up to distance 24. In this way we do not need any unphysical criteria for determining β_c, but we just have to monitor variations of physical quantities (such as ξ or the order parameter itself).

Let us define

$$C(z) = \left\langle \frac{1}{L_x L_y} \operatorname{Re} \sum_{x,y} P(x,y,z) \right\rangle. \tag{2}$$

For L_z going to infinity, we know that

$$C(z) \underset{z \to \infty}{\to} A e^{-mz} + B, \tag{3}$$

where B is the value of the real part of the Polyakov loop at a large distance from the wall, i.e., the *spontaneous magnetization*, which is zero in the symmetric phase. The *mass* m is the inverse of ξ or, in terms of σ, $m = \sigma L_t$. With our boundary conditions the exponential in (3) has to be replaced by $\cosh[-m(\frac{1}{2}L_z - z)]$.

We use the *smearing procedure*[8] to generate operators weakly coupled to the high-energy fluctuations. Moreover we use the independence of the extrapolated *mass* from the smearing number as an indication of a large-z asymptotic behavior. With this technique we construct progressively larger operators which have the same transformation properties under Z_3.

The smearing procedure is very useful, but time consuming. The situation worsens at large β or close to β_c, where it is necessary to carry out a large number of smearing steps in order to get an optimal projection over the ground state. This problem can be alleviated very easily. After s smearing steps, in the measure process at a given z, we can transform the tridimensional lattice into a smaller one ($\frac{1}{2}L_x \times \frac{1}{2}L_y \times \frac{1}{2}L_t$) by the blocking transformation:

$$U_\mu^{(s+1)}(\mathbf{N};z) = U_\mu^{(s)}(2\mathbf{n};z) U_\mu^{(s)}(2\mathbf{n}+\mu;z),$$

where $\mathbf{n} = (x,y,t)$, μ is an unitary vector in the x, y, or t direction, and $U^{(s)}$ is the s-times smeared link. $\mathbf{N}$ denotes a point on the coarse-grained lattice, which is 8 times smaller than the original one. After this step we continue with the usual smearing procedure done on the fields defined on the coarse-grained lattice. We will use the index s to denote the quantities defined in (1) and (2) when they are calculated by using the $U^{(s)}$ variables. We have carried out just one smearing step on the original lattice, and after the blocking procedure described above, nine more smearing steps on the blocked lattice.

This computation required about 4500 hours on a 256-Mflops Ape computer.[9] We used an overrelaxed method[10] for updating the gauge fields. We have done some test runs by using the Metropolis and the quasi-heat-bath methods, and the results are fully compatible.

We have used two different lattice sizes: $8^2 \times 32 \times 4$

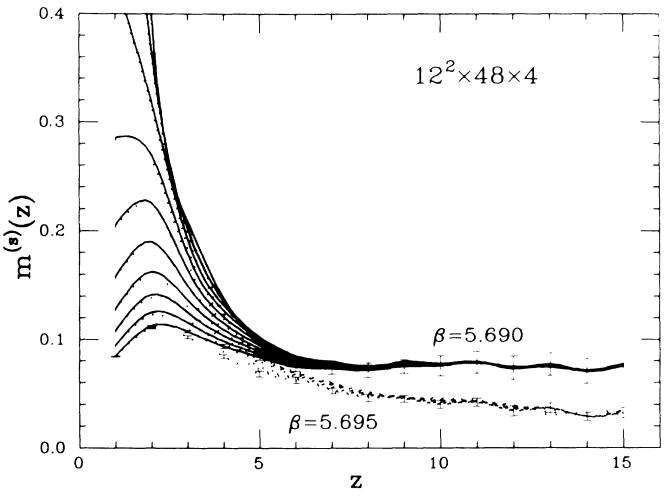

FIG. 1. $m^{(s)}(z)$, see Eq. (4). Every line corresponds to a given s. The error bars are displayed for $s=11$. The finiteness of B at $\beta=5.695$ is reflected in a decrease of $m^{(s)}(z)$ for large z.

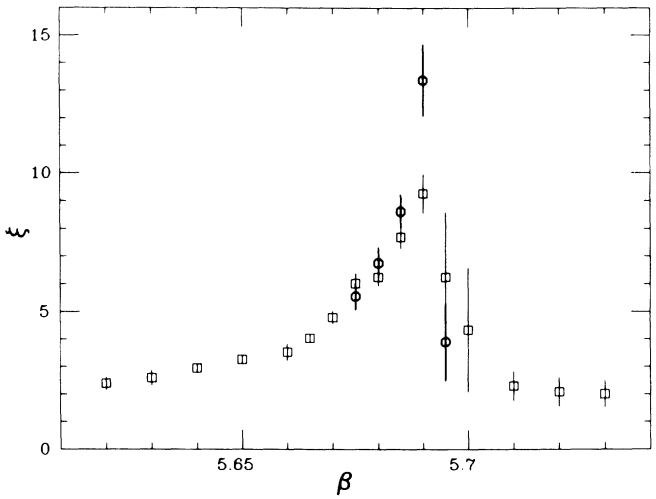

FIG. 2. Results for ξ. The squares correspond to the $8^2\times32\times4$ lattice and the circles to the $12^2\times48\times4$ one.

and $12^2\times48\times4$. For each β in the smaller (larger) lattice we have run up to 170000 (240000) iterations discarding 7000 (10000) for thermalization. Measures have been taken every ten sweeps. For error calculations we have considered subsamples of 10000 iterations as independent measurements. Close to β_c we find a very strong slowing down, with correlations up to the order of 10000 MC iterations.

The first analysis (method I) that we consider is based on the effective masses as computed from operators of a given smearing number s:

$$m^{(s)}(z)=\ln\left[\frac{C^{(s)}(z)}{C^{(s)}(z+1)}\right] \tag{4}$$

(or the generalization for a hyperbolic-cosinus behavior). When $B=0$ the effective mass approaches $1/\xi$ when $z\rightarrow\infty$. Conversely the behavior of $m^{(s)}(z)$ for large z is very sensitive to a nonzero B, allowing an accurate determination of β_c.

A second analysis (method II) is carried out by means of global fits, discarding a large number of points in the neighborhood of the wall, and fitting the remaining ones to a three-parameter function: $A\cosh[m(\frac{1}{2}L_z-z)]+B$.

First, we need a precise determination of β_c. To do that we have used two independent criteria. An application of the method I is shown in Fig. 1. We clearly distinguish for $\beta=5.695$ the presence of spontaneous magnetization (i.e., $B\neq0$), while at $\beta=5.690$ we have not found any sign of it. The presence of spontaneous magnetization can also be directly computed with a three-parameter global fit (method II).

The precise determination of ξ in the neighborhood of β_c is the main result of this paper. We note that all the quantities computed with both methods are perfectly compatible. The large ξ that we have measured in this work (up to thirteen lattice units) is only accessible when high statistics and improved techniques are used. We have checked that when only small values of z are accessible and the smearing procedure is not used, a smaller ξ is found, and then the transition might appear as a first-order one. Also, close to β_c, if the statistics is poor (and L_z short), one can mistake a slowly decreasing signal for the effects of a spontaneous magnetization.

In Fig. 2 and in Table I we summarize the results for ξ. We found ξ as large as the transversal dimension L_x, in both lattices, which is the behavior we expect in a second-order transition, since in this case the lattice size is the only bound for ξ. This is an indication of a divergence in this quantity at β_c in the thermodynamical limit. At β_c the relation that we found between ξ in the two lattices is 1.42(18) in agreement with the predicted value $\frac{12}{8}=1.5$ in a second-order phase transition. Preliminary

TABLE I. Results for ξ in lattice units, from the analyses I and II.

β	$\xi^{(I)}$	$\xi^{(II)}$
	$8^2\times32\times4$ lattice	
5.675	6.0(4)	5.9(7)
5.680	6.3(3)	6.1(6)
5.685	7.7(4)	7.7(7)
5.690	9.3(7)	8.8(1.1)
5.695	...	6.2(2.3)
	$12^2\times48\times4$ lattice	
5.675	5.6(5)	5.1(7)
5.680	6.8(6)	6.3(8)
5.685	8.6(6)	9.0(1.4)
5.690	13.4(1.3)	13.0(1.9)
5.695	...	3.9(1.3)

results[6] at $\beta=5.690$ in a $16^2\times64\times4$ lattice confirm that $B=0$ and also show an increase of ξ.

Our data conclusively show that ξ strongly increases when we move toward the transition. We have not observed any evident sign of discontinuities. At the transition, ξ increases as the transverse dimension of the lattice and it is at least $3/T_c a$ in the largest lattice that we have considered. It is quite evident that data taken on a lattice which is smaller than ξ cannot be used in an argument for a first-order transition. Therefore, most of the published conclusions on the order of the transition should be reconsidered.

All of our data seem to show the existence of a second-order phase transition, and no indications are found for a first-order one. We stress, however, that it is not impossible that a first-order transition happens when ξ is very large (i.e., a weak first-order transition), but if this were the situation in pure QCD, and the physical correlated lengths were so large at the critical temperature, this could be decided only by carrying out computations on a much larger lattice. For the time being our data exclude the existence of the strong first-order phase transition which was claimed in the literature.

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