Deconfining Phase Transition in Lattice QCD

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We present the first results obtained from the sixteen-processor version of the parallel supercomputer being built at Columbia. The color-deconfining phase transition has been studied for pure SU(3) gauge theory on lattices with a spatial volume of 16^3 sites and temporal sizes of 10, 12, and 14 sites. The values found for the critical coupling are 6.07, 6.26, and 6.36, respectively. These results are in agreement with the perturbative predictions of the renormalization group, suggesting that lattice QCD calculations with the parameter β at least as large as 6.07 may approximate the continuum limit.

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The question of how small the lattice spacing a must be in order to reproduce continuum physics is presently one of the most important in lattice QCD. In the continuum limit, the renormalization group predicts that a, when measured in physical units, decreases in a known way as the bare coupling g approaches zero. If one uses the critical temperature T_c of the color-deconfining phase transition to determine the physical scale, then one can study this question by comparing the numerically calculated g dependence of the product $T_c a$ with that predicted by the continuum renormalization group:

$$T_c a = c\beta^{51/121}\exp(-4\pi^2\beta/33). \quad (1)$$

Here β is defined as $6/g^2$, and c is a constant that is not determined by perturbation theory.

Although the earliest work[1] on lattices with two and four sites in the temporal direction showed a scaling behavior in agreement with Eq. (1), more recent results[2] on larger lattices are inconsistent with the continuum perturbation predictions of Eq. (1). In Fig. 1 we show both these earlier results and the values reported in this paper from still larger lattices. The curve shown for comparison has a slope given by Eq. (1) but a y intercept determined by fitting the constant c to our three points.

Let us recall the conventional picture of the color-deconfining phase transition in lattice QCD. The partition function is given by

$$Z = \int \prod_l dU_l \exp\left(-\frac{2}{g^2}\sum_P \mathrm{Re}\,\mathrm{tr}(I - U_P)\right),$$

where U_l is the element of SU(3) associated with the link l, and U_P is the product of the links around the plaquette P. A calculation performed on a $N_s^3 \times N_t$ lattice can be interpreted as representing a system with a finite volume $V = (aN_s)^3$ at a temperature $T = 1/(aN_t)$. For sufficiently large N_t (i.e., at sufficiently low temperature T) one finds the usual confinement of color charge. However, as the number of lattice sites in the time direction is decreased, a critical value $N_{tc} = 1/aT_c$ is reached below which color charge is no longer confined. This high-temperature region is characterized as a gluon plasma phase in which color charge is screened but not confined. Both phases are of considerable physical interest: The low-temperature phase describes the usual QCD vacuum and the high-temperature phase corresponds to a physical environment which may be created in the collision of high-energy nuclei and possibly realized at an early stage in the evolution of the universe.

These two phases are usually distinguished in Monte Carlo calculations by examination of the expectation value of the Polyakov loop operator $P(x)$,

$$P(x) = \mathrm{tr}(\prod U_l)/3, \quad (2)$$

constructed for each spatial coordinate x by taking the trace of the product of the link variables U_l associated with the line L of links in the time direction with spatial coordinate x. The operator $P(x)$ is a component of the color-vector potential [written as a matrix in the fundamental representation of SU(3)] along the line L. This operator describes the insertion of a massive color-triplet source (quark), with world line L, into the interacting system of gluons. In the low-temperature, confining phase such an isolated quark will have an in-

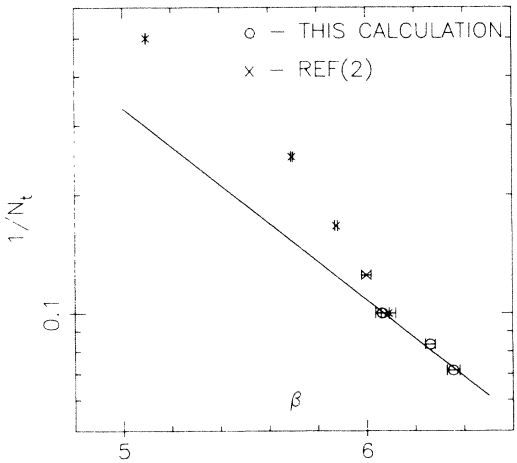

FIG. 1. The product of critical temperature and lattice spacing plotted as a function of the parameter $\beta = 6/g^2$. The curve has the slope predicted by continuum perturbation theory. Its y intercept is fitted to the large-lattice data.

finite energy so the expectation value of $P(x)$ should vanish. In contrast, for $T > T_c$, $P(x)$ should have a nonvanishing expectation value.

In the lattice version of the theory, this phase transition is related to the breaking of a global Z(3) symmetry for which the operator $P(x)$ represents an order parameter. This symmetry consists of multiplying all of the timelike links in a single time plane by the same element z of the center of the gauge group. Under this transformation $P(x) \rightarrow zP(x)$. This Z(3) symmetry implies that there should be three possible expectation values of $\langle P(x) \rangle$, related by multiplication by the elements of Z(3). In fact, it can be argued[3] that $P(x)$ should be simply proportional to the elements of Z(3). Such a phase transition is expected[3] to be first order, a conclusion supported by the previous numerical work.[1,2]

Use of $\langle P(x) \rangle$ to distinguish the confined and deconfined phases in actual calculations poses two difficulties, which become more severe as we approach the continuum limit. First, in the limit of large N_t, the expectation value of $P(x)$ in the deconfined phase vanishes exponentially in N_t. This is a consequence of the linear divergence ($\sim 1/a$) in the self-energy of a pointlike color charge.

The second problem arises from the Z(3) symmetry described above. The integration of $P(x)$ over the Z(3) transforms of each gauge configuration causes the expectation value of $P(x)$ to vanish. By analogy with the Abelian gauge theory, this vanishing of $\langle P(x) \rangle$ can be viewed as following from the integrated form of Gauss's law which forbids a net charge in a finite volume with periodic boundary conditions. Thus if one averages over very long Monte Carlo runs in order to measure the necessarily small quantity $\langle P(x) \rangle$, these global changes in phase will occur, causing $\langle P(x) \rangle$ to vanish even in the deconfined phase.

Of course, in the limit of infinite volume a single isolated charge is no longer inconsistent with Gauss's law and these changes of phase extending over the entire volume become impossible. To see deconfinement in a finite system, one must limit the length of the Monte Carlo averages to avoid averaging over these Z(3) transformations and hence restrict the precision with which $\langle P(x) \rangle$ can be determined. This situation is typical of finite-volume calculations of an order parameter in a phase with spontaneous symmetry breaking.

Now let us turn to the details of our calculation. Since N_t cannot be varied continuously, it is convenient to vary $N_{tc} = 1/T_c a$ by varying the parameter β. We search for the critical value of β at which N_{tc} equals the value of N_t for the lattice on which we are working. For each of our three values of N_t, we have performed runs of 10 000 to 20 000 sweeps for four or five values of β in the region of the phase transition. For each sweep we calculated the real and imaginary parts of all Polyakov loop operators, and the spacelike and timelike plaquettes. All four quantities were averaged over the lattice.

For each value of β, we began with all link variables equal to the identity matrix. The first 1000 sweeps were then discarded to eliminate effects due to incomplete thermalization. Increasing the number of sweeps discarded had no systematic effect on the mean value or the fluctuations in any of the quantities which we calculated.

For temperatures not too close to the transition, the phase of the system can be easily determined by look-

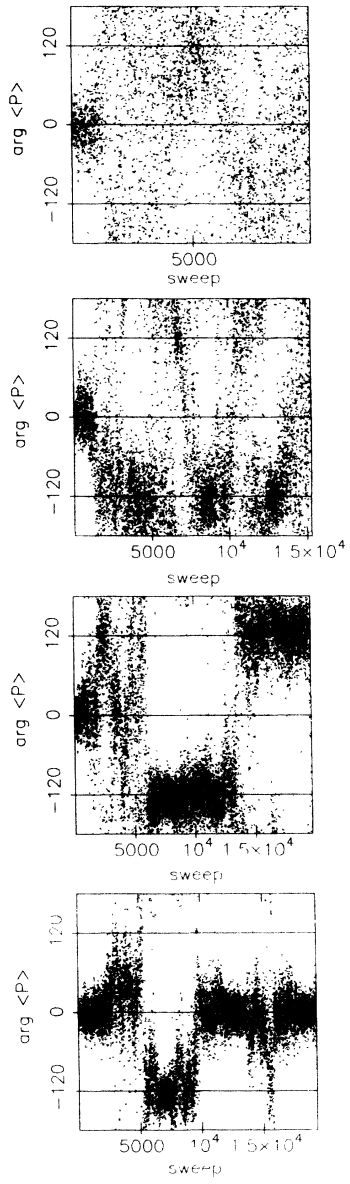

FIG. 2. The argument of $\langle P \rangle$ vs sweep for $N_t = 14$ and $\beta = 6.2$, 6.3, 6.4, and 6.5. The average is carried out over the volume for each sweep.

ing at the Monte Carlo evolution of the argument of $P(x)$ averaged over the lattice for a single sweep (see Fig. 2). Below the transition, the magnitude of $\langle P \rangle$ is small and its argument appears to be random, with large changes in value from sweep to sweep. Above the transition, the magnitude of $\langle P \rangle$ is significantly larger and the argument stays within a band around one of the cube roots of unity for many hundreds of sweeps, with relatively quick jumps from one of the Z(3)-equivalent phases to another. This tunneling corresponds to the integration over the center of the group which imposes Gauss's law as discussed above.

Near the phase transition, the jumps between these bands occur more frequently but take longer to complete, with more time being spent in a region of ambiguous phase. Thus at intermediate values of β we see a mixture of the two limiting types of behavior, corresponding to the existence of the two phases and indicating the first-order nature of the transition. The finite width of the interval in β (typically 0.2 or 0.3) over which we see both behaviors reflects the finite-size rounding that should be expected from a calculation performed in a relatively small physical volume.

As discussed above, we compute $\langle P \rangle$ by averaging over both the spatial volume and blocks of Monte Carlo sweeps. We must limit the number of sweeps in a block so that a spontaneous Z(3) rotation in the deconfined phase is unlikely to occur. In the limit of infinite volume, the block size could become arbitrarily large and we would have a proper Monte Carlo average. For our finite-volume calculation, this procedure results in a number of independent, but completely averaged, values of $\langle P \rangle$ which can be studied. Figure 3 shows scatter plots of the complex values of $\langle P \rangle$ computed for the block size of 100 which we have used.

In order to proceed quantitatively, we must introduce a procedure to define β_c which can be applied even when finite-volume rounding is present. As is evident from the scatter plot in Fig. 3, the angular distribution of the blocked quantity $\langle P \rangle$ provides the sharpest differentiation between the confined and deconfined phases. We proceed as follows: For each value of N_t and β, we superimpose the three symmetrical 120° sectors so that for each of the blocked averages $\langle P \rangle$ we obtain an angle ϕ in the range between $+60°$ and $-60°$. The resulting distribution of angles is shown in the histograms of Fig. 4 for $N_t = 14$.

Below the transition, the distribution is essentially flat while above the transition, it has a sharp peak at $\phi = 0$. For all three values of N_t, this peak was contained within a region between $+20°$ and $-20°$. Thus if we define the blocks with angles lying outside this 40° region as corresponding entirely to the confined phase, we can compute the fraction $f(\beta)$ of our complete sample which is confined. The statistical uncertainty in $f(\beta)$ can be determined precisely knowing

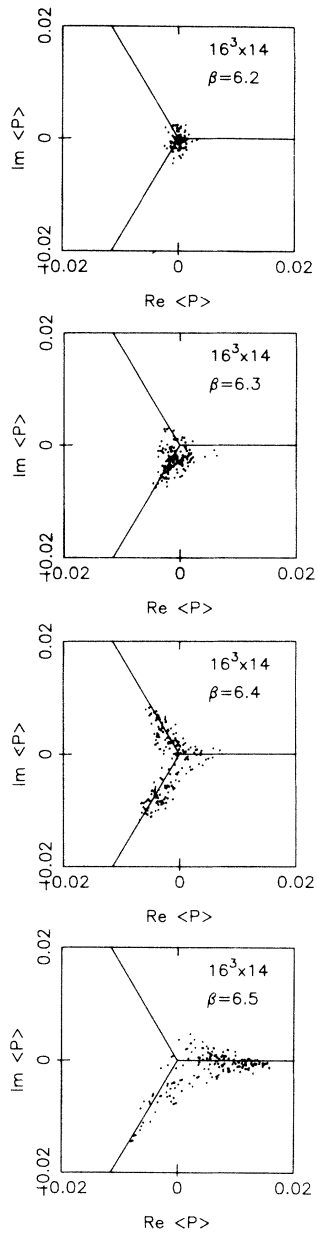

FIG. 3. Scatter plots for $\langle P \rangle$ averaged over blocks of 100 sweeps.

the number of blocks lying outside the 40° region and taking into account the autocorrelation in our sample.

A linear interpolation between the values of β which have $f(\beta)$ bracketing $\frac{1}{2}$ gives our critical value of β with $f(\beta_c) = \frac{1}{2}$. This method[4] represents a reasonable (if somewhat arbitrary) definition of the critical coupling strength in the presence of finite-volume rounding of the phase transition. It has the virtue of providing a definite value of β_c with well-defined errors which can be used to extrapolate to the infinite-volume limit.

Our results are presented in Table I together with the predictions of Eq. (1) choosing the constant c to

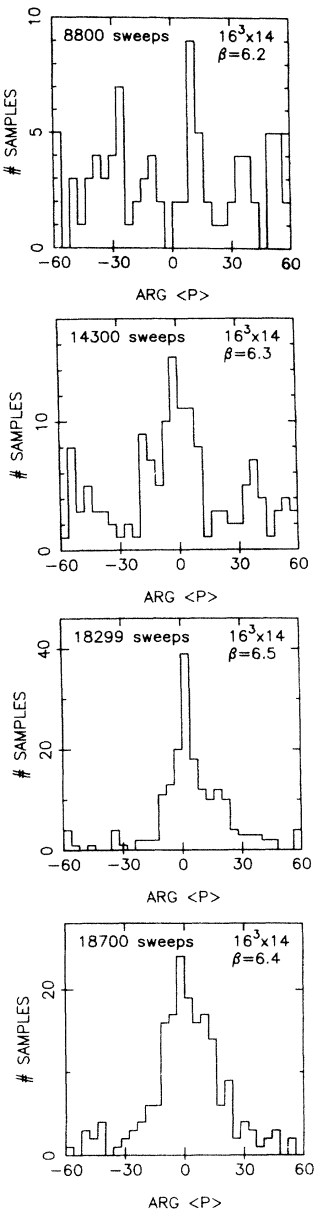

FIG. 4. Histograms showing the distribution of arguments of $\langle P \rangle$ averaged over blocks of 100 sweeps, for $N_t = 14$ and $\beta = 6.2$, 6.3, 6.4, and 6.5.

give a best fit. We have studied the sensitivity of these results to our analysis procedure by increasing the width of the region excluded when calculating $f(\beta)$ to $\pm 30°$ and the block size to 200 sweeps. Both of these changes increased the errors but gave results consistent with those in the table. As can be seen, our results are in very good agreement with the predictions of the perturbative, continuum renormalization group.[5]

This calculation was carried out on a sixteen-processor supercomputer designed and built for lattice-gauge-theory calculations.[6] The processors are connected in a 4×4 rectangular mesh, with direct communication provided between nearest-neighbor pairs of processors. Each processor consists of an Intel 80286 microprocessor, coupled to a high-performance 22-bit floating-point multiplier-accumulator. The time required to update a link was 180 μs, using a ten-hit Metropolis program which reunitarized the link variables after each sweep.

TABLE I. Values for β_c with statistical errors and the predictions of Eq. (1) with $c = 67.3 \pm 1.0$. This value of c corresponds to $T_c/\Lambda_L = c(33/8\pi^2)^{121/55} = 46.6 \pm 0.7$.

N_t	β_c	Scaling
10	6.065 ± 0.027	6.08
12	6.261 ± 0.020	6.24
14	6.355 ± 0.026	6.38

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[5]This comparison with scaling is strictly valid only if the spatial volumes have been scaled by the ratio of the cubes of N_t. Although this condition is not met for our calculation, the volume dependence found on smaller lattices by Kennedy *et al.* (Ref. 2) suggests that the change in volume which should have accompanied a change in N_t from 10 to 14 corresponds to a change in β_c of 0.03, which is comparable to our statistical errors.

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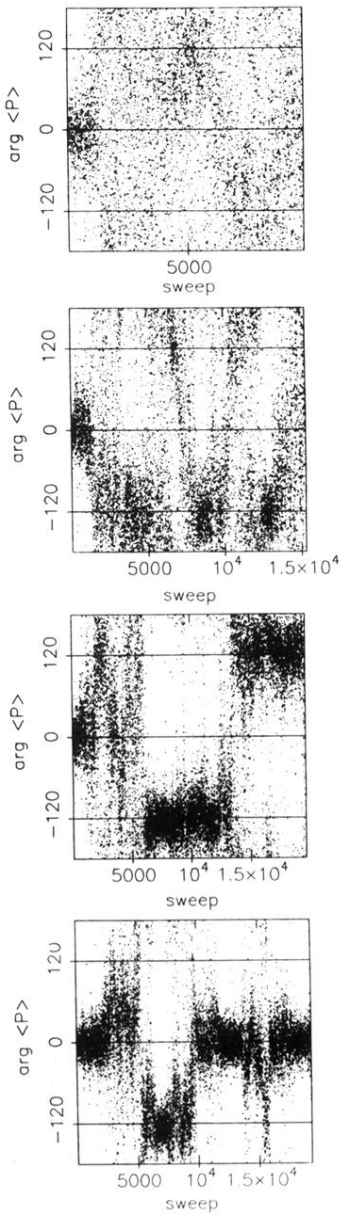

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