Deconfining Transition of SU(3) Gauge Theory on $N_t = 4$ and 6 Lattices

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We report the results of a Monte Carlo study of finite-temperature pure SU(3) gauge theory performed on the parallel computer QCDPAX. The deconfining transition is studied on $12^2 \times 24 \times 4$, $24^2 \times 36 \times 4$, $24^3 \times 6$, and $36^2 \times 48 \times 6$ lattices with $480\,000-1\,112\,000$ iterations. A clear two-phase structure is observed on spatially large $(24^2 \times 36 \times 4 \text{ and } 36^2 \times 48 \times 6)$ lattices and the gaps of physical quantities at the transition are calculated on these lattices. The latent heat thus obtained on the $N_t = 6$ $(36^2 \times 48 \times 6)$ lattice is much smaller than the one previously obtained.

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Numerous works have been devoted to the study of the finite-temperature deconfining phase transition of lattice QCD. Recently, it has been realized that the determination of the nature of the transition requires much more intensive numerical calculations than done previously even in pure SU(3) gauge theory [1]. Through the studies on the $N_t = 4$ (N_t is the lattice size in the temporal direction) lattices with large spatial volume and with high statistics, now the order of the phase transition has been definitely determined to be first order [2-4]. It has also turned out that the latent heat calculated on the $N_1 = 4$ lattices is much smaller than previously determined [2]. The latent heat in pure gauge theory is one of the fundamental quantities in lattice QCD, although the real value which can be used in the studies of the early Universe and heavy-ion collisions should be calculated in full QCD. Thus in this Letter we study the deconfining transition in pure SU(3) theory, in particular, the latent heat on the $N_t = 6$ lattice, by a precise calculation. Of course, $N_t = 6$ is too small to obtain the continuum limit of the latent heat. Nonetheless we hope that this is a step towards the continuum limit.

The calculation has been done on the massively parallel computer QCDPAX [5], a MIMD (multiple instruction, multiple data) machine constructed at the University of Tsukuba as the fifth generation of PAX (parallel array experiment) [6] computers. QCDPAX is a 14 Gflops machine with 480 nodes.

We first study the $N_t = 4$ system $(12^2 \times 24 \times 4 \text{ and } 24^2 \times 36 \times 4 \text{ lattices})$ with statistics which are largely improved compared with the previous works. As is shown below, we obtain results which are completely consistent with the previous results and furthermore we obtain new results such as a clear four-peak structure of the Polyakov loop at the deconfining temperature. Therefore we are convinced that the hardware and software of QCDPAX are working perfectly. Then we further study $N_t = 6$ lattices with large spatial volume $(24^3 \times 6 \text{ and } 12^3 \times 6 \text{ and } 12$

 $36^2 \times 48 \times 6$ lattices) in high statistics. A preliminary result of a part of this work has been reported in Ref. [7].

Using the standard one-plaquette action, the gauge configurations are updated with a three SU(2) subgroup eight-hit pseudo-heatbath algorithm. The acceptance rate is about 95%. At every iteration we measure spatial and temporal plaquettes as well as the spatially averaged Polyakov loop Ω . The one-link update time for full size QCDPAX with 480 nodes is 1.44 μ sec.

For the $N_t = 4$ case, we perform 712000 Monte Carlo iterations on the $24^2 \times 36 \times 4$ lattice at $\beta = 5.6925$ and 910000 iterations on the $12^2 \times 24 \times 4$ lattice at $\beta = 5.6915$. As is shown below, these β values exactly agree with the deconfining transition points β_c within statistical errors. These statistics are much improved over the previous works (see Ref. [1]). For the $N_t = 6$ case, the Columbia group [2] reported the results of 10000-100000 iterations at several values of β on $(16^3 - 24^3) \times 6$ lattices. Here, we perform 480000 iterations on the $24^3 \times 6$ lattice at $\beta = 5.89$ and 1112000 iterations on the $36^2 \times 48 \times 6$ lattice at $\beta = 5.8936$. Note that the spatial lattice size is greatly enlarged and that the statistics are one order improved compared with the previous work for the case of the $36^2 \times 48 \times 6$ lattice.

We can see many flip-flops in the histories of the average plaquette on all the lattices, as is shown in Fig. 1 for



FIG. 1. Average plaquette histories on the $36^2 \times 48 \times 6$ lattice at $\beta = 5.8936$.

the case of the $36^2 \times 48 \times 6$ lattice. The histogram of the absolute value of the Polyakov loop on the spatially large lattices $(24^2 \times 36 \times 4 \text{ and } 36^2 \times 48 \times 6)$ shows a clear double-peak structure and furthermore the histogram of the Polyakov loop on the complex plane shows a four-peak structure (see Fig. 2 and Ref. [7]). These are consistent with the first-order phase transition associated with the spontaneous breakdown of the Z(3) symmetry.

The many flip-flops seen in the histories allow us to apply the spectral density method [8] to see the β dependence of observables near the simulation point. The main purpose of this analysis is to get a precise location and the properties of the phase transition. We study the susceptibility χ of the real part of the Z(3)-rotated Polyakov loop Ω_{rot} and that of the averaged plaquette *P*:

$$\chi_{\mathcal{F}} \equiv V(\langle \mathcal{F}^2 \rangle - \langle \mathcal{F} \rangle^2) ,$$

where $\mathcal{F} = \Omega_{rot}$, *P*. Here and in the following, we denote the spatial volume of the lattice as *V*. The peak position of the susceptibility is identified with a finite-volume estimate of the transition point β_c .

Errors are estimated using the jackknife method [9]. The bin-size dependence of the estimated errors is studied to remove the autocorrelation effects. The large statistics of our data allows us to vary the bin size widely. From this study we find that large numbers are required for the bin size to get reliable values of errors which are stable for an increase of the bin size: We use the bin size of 35500 (50000) for observables averaged over both the confining phase and deconfining phase on the $24^2 \times 36 \times 4$ ($36^2 \times 48 \times 6$) lattice. As expected, these bin sizes are comparable with the average persistent time of the phases seen in the histories. For quantities in each phase, the required bin sizes are smaller, typically 3000-5000.

The results for $\chi(\Omega_{rot})$ are shown in Fig. 3. Note that our β 's are located exactly at the transition point except for the case of the $24^3 \times 6$ lattice. Figure 4 summarizes our results ($N_t = 4$ and 6) for the peak height χ_{max} and the peak position β_c of the susceptibility together with the results of the Kyoto-Tsukuba collaboration for $N_t = 4$ [4].

The finite-size scaling predicts a linear scaling law $\chi_{\max}(V) \sim V^{\rho}$ and $\beta_c(N_t, V) - \beta_c(N_t, \infty) \sim V^{-\sigma}$ with $\rho = \sigma = 1$ for first-order transitions, in contrast with non-trivial critical exponents of second-order transitions. A power-law fit using lattices of $N_t = 4$ and $V/N_t^3 > 50$ (including the Kyoto-Tsukuba data) leads to

$$\chi_{\Omega,\max} = 0.1070(75) (V/N_t^3)^{1.038(15)}$$

resulting in a critical exponent ρ very close to unity. Allowing an extra constant term in the fit leads to $\rho = 1.05(27)$. Thus the results are completely consistent with the previous conclusion [1] that the deconfining transition is first order.

We estimate the infinite-volume limit of β_c , assuming $\sigma = 1$. Using the lattices $V/N_t^3 > 50$, we find

$$\beta_c(4,V) = 5.69247(23) - 0.053(26)N_t^3/V$$



FIG. 2. Polyakov loop histograms on the $36^2 \times 48 \times 6$ lattice at $\beta = 5.8936$: (a) $|\Omega|$ and (b) Ω on the complex plane.



FIG. 3. Susceptibility of the Z(3)-rotated Polyakov loop: $\chi(\Omega_{rot})/V$. (a) $N_t = 4$; (b) $N_t = 6$.



FIG. 4. (a) Peak height and (b) peak position of $\chi(\Omega_{rot})$ as a function of relative spatial volume V/N_t^3 . Open circles are the data on the $N_t = 4$ lattices by the Kyoto-Tsukuba collaboration. Solid circles and squares are our results on the $N_t = 4$ and 6 lattices, respectively.

and

$$\beta_c(6,V) = 5.89405(51) - 0.072(77)N_t^3/V$$

The resulting $\beta_c(4,\infty)$ is consistent with the estimate of the Kyoto-Tsukuba group: 5.69226(41). Our $\beta_c(6,\infty)$ is significantly larger than a previous estimate [10] of 5.877(6) extrapolated from small lattices: $V = 7^3 - 11^3$.

Comparing the N_t dependence of our $\beta_c(N_t,\infty)$ with the prediction of a two-loop perturbation theory for the shift of β_c , $\Delta\beta_{2\text{-loop}}$, we find $[\beta_c(6,\infty) - \beta_c(4,\infty)]/\Delta\beta_{2\text{-loop}} = 0.561(2)$. This asymptotic-scaling violation was noted in previous works [10], and the magnitude of the violation is consistent with previous estimates by the Monte Carlo renormalization-group (MCRG) method at these β 's [11].

Now let us study gaps of thermodynamic quantities at the phase transition. We expect a finite gap (latent heat) for the energy density ϵ but no gap for the pressure p. Conventionally, combinations $\epsilon - 3p$ and $\epsilon + p$ are studied, because they are proportional to a sum and a difference of the spacelike and timelike plaquette averages, P_s and P_t , respectively [12]:

$$\epsilon - 3p = -36[\beta(g)/g^3](P_t + P_s),$$

$$\epsilon + p = 4\beta c(\beta)(P_t - P_s).$$

TABLE I. $(\epsilon - 3p)/T^4$ and $(\epsilon + p)/T^4$ with one-loop perturbative coefficients assumed. Phase separation is performed as explained in the text.

$\frac{\text{Lattice}}{\beta}$	24 ² ×36×4 5.6925	36 ² ×48×6 5.8936
$(\epsilon + p)_{had}/T^4$	0.508(47)	0.360(35)
$(\epsilon + p)_{OGP}/T^4$	3.324(29)	2.195(37)
$(\epsilon - 3p)_{\text{had}}/T^4$	703.478(74)	3776.892(43)
$(\epsilon - 3p)_{OGP}/T^4$	707.539(42)	3779.287(46)
$\Delta(\epsilon + p)/T^4$	2.773(55)	1.835(51)
$\Delta(\epsilon - 3p)/T^4$	4.062(85)	2.395(63)

Here $\beta(g)$ is the renormalization-group beta function and $c(\beta)$ is a response function of the gauge coupling constant with respect to the asymmetry deformation of the lattice. In the perturbation theory they are given by

$$-36\beta(g)/g^3 = 99/\pi^2 + O(\beta^{-1})$$

and

$$c(\beta) = 1 - 1.00062\beta^{-1} + O(\beta^{-2})$$

We calculate the gaps on the $24^2 \times 36 \times 4$ and $36^2 \times 48 \times 6$ lattices: On these lattices, our β 's locate exactly at the transition points, as mentioned earlier, and twophase structure is very clear both in the history and in the histogram, as Figs. 1 and 2 show. In order to obtain the energy gap at the transition, we have to separate the Monte Carlo runs at the transition into two phases. We find that, as mentioned in Ref. [4], the separation of a run into two phases by an inspection of the time history of the Polyakov loop is stable, if we disregard a large enough number of iterations around the flip-flops: We disregard 2000 (3000) iterations around the flip-flops for the $24^2 \times 36 \times 4$ ($36^2 \times 48 \times 6$) lattice.

Our results for $(\epsilon - 3p)/T^4$ and $(\epsilon + p)/T^4$ with perturbative coefficients assumed are summarized in Table I [13]. These results can be compared with the previous ones: On the 24³×4 lattice at the same β , $\Delta(\epsilon - 3p)/T^4 = 4.200(95)$ (Kyoto-Tsukuba [4]), 3.78(20) (Columbia [2]); and $\Delta(\epsilon + p)/T^4 = 2.927(97)$ (Kyoto-Tsukuba), 2.54(12) (Columbia). On the 28³×4 lattice at $\beta = 5.692$, $\Delta(\epsilon - 3p)/T^4 = 4.11(12)$ and $\Delta(\epsilon + p)/T^4 = 2.826(37)$ (Kyoto-Tsukuba). Note that our results for $N_t = 4$ are completely consistent with those of the Kyoto-Tsukuba group: The values of the physical quantities in both the phases themselves agree with each other.

For $N_t = 6$, the Columbia group estimated $\Delta(\epsilon + p)/T^4 = 2.48(24)$ on the $24^3 \times 6$ lattice. We find a much smaller value, 1.835(51), for this gap (see Table I). We understand the origin of the discrepancy as follows: (1) The Columbia group measured $(\epsilon + p)/T^4$ in the deconfining phases at $\beta = 5.9$ which is slightly above our estimate of $\beta_c = 5.8938(3)$ and obtained [14] 2.60 which is larger than our value 2.195 at $\beta = 5.8936$ by 0.405. This difference can be attributed to the sharp drop in

 $(\epsilon + p)/T^4$ above the transition point observed by the Columbia group. (2) The value of $(\epsilon + p)/T^4$ in the confining phase assumed by the Columbia group [14] is 0.12 at $\beta = 5.875$ which is smaller than our value 0.36 by 0.24. Our data indicate that the increase of $(\epsilon + p)/T^4$ in the confined phase near β_c in the data of the Columbia group, which they took as due to mixing of the phases, is partly a real effect. Thus these two facts in total lead to the difference of 0.645 (=2.48 - 1.835) for the gap.

These results raise two problems: First, gaps for $N_t = 6$ are smaller than those for $N_t = 4$ by a factor 1.5 for $\Delta(\epsilon+p)$ and 1.7 for $\Delta(\epsilon-3p)$, indicating naively a scaling violation at these values of β . Second, both $N_t = 4$ and $N_t = 6$ results show discrepancies between $\Delta(\epsilon-3p)$ and $\Delta(\epsilon+p)$, which again naively suggests a finite pressure gap at the transition.

Since the violation of the asymptotic scaling at these β 's is already well established [11], the use of perturbative coefficients for $\epsilon - 3p$ and $\epsilon + p$ is not validated and we have to estimate nonperturbative corrections to these quantities.

Because the coefficient of $\epsilon - 3p$ is given by the beta function, we can apply to it the nonperturbative beta function obtained by studies of MCRG and the deconfining phase transition. The correction factor to the oneloop perturbative beta function which the MCRG studies [11] give is 0.6 ± 0.05 at $\beta \approx 5.7$ and 0.75 ± 0.07 at $\beta \approx 5.9$. Large error bars are caused by the dispersive MCRG results. (A similar approach was also proposed by Engels *et al.* [15].) These corrections make $\Delta(\epsilon - 3p)/T^4 = 2.44 \pm 0.24$ for $N_t = 4$ and 1.43 ± 0.14 for $N_t = 6$. Therefore even after we include the correction factors, the discrepancy between the two still remains. Thus $\Delta(\epsilon - 3p)/T^4$ shows a substantial scaling violation at these β 's.

Now the differences between the corrected $\Delta(\epsilon - 3p)/T^4$ and the uncorrected $\Delta(\epsilon + p)/T^4$ are small for both the $N_t = 4$ and $N_t = 6$ lattices. Since we expect that Δp is zero, this suggests that nonperturbative correction to the coefficient of $\epsilon + p$ is small. The confirmation of this requires a numerical study of anisotropic lattices [16] with small anisotropy.

We have performed precise measurements of the deconfining transition in pure gauge theory on the dedicated machine QCDPAX. After confirming the first-order nature of the transition, we have found that the latent heat on the $N_t = 6$ lattice is much smaller than that on the $N_t = 4$ lattice and $\frac{1}{3} - \frac{1}{4}$ of the Stefan-Boltzmann value $15/8\pi^2$. Whether this small value of the latent heat continues to the continuum limit is an important question left for further investigations. We are very grateful to A. Ukawa for valuable discussions, helpful suggestions, and reading of the manuscript, and to N. Christ for sending us their numerical data. We also thank M. Fukugita, J. Engels, A. Nakamura, and S. Sakai for useful discussions and suggestions. This project is supported by the Grant-in-Aid of Ministry of Education, Science and Culture of the Japanese Government (No. 62060001 and No. 02402003).

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