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Abstract

We explore how spectral density reweighting techniques can be applied to the analysis of the chiral phase transition in finite-temperature Quantum Chromodynamics (QCD). We consider lattice QCD with 4 flavors of dynamical staggered fermions and $m_q a = 0.025$. Our simulations were performed using the Hybrid Monte Carlo method for $L_t L^3$ lattices, with $L_t = 4$ and $L = 6, 8$ and 10 . We calculate partition function zeros, as well as the maxima of the specific heat and of the susceptibilities for the Polyakov loop and for the chiral condensate. A finite size scaling analysis of these data leads to preliminary results for the critical coupling β_c , for the critical exponent ν , for the latent heat, and for the jumps in the Polyakov loop and in the chiral condensate.

The temperature phase structure of Quantum Chromodynamics (QCD) is one of the main problems we are faced with in theoretical investigations of the properties of strongly interacting matter. Since it is due to non-perturbative phenomena, its study requires a well defined approach valid beyond perturbation theory. Universality arguments lead us to expect the following phase diagram depending on the temperature and the current quark mass m_q . In the quenched limit ($m_q \rightarrow \infty$), the dynamics of QCD reduces to that of pure SU(3) theory, where a first order phase transition takes place: from the Z_3 -symmetric confined phase, where the only physical degrees of freedom are glueballs, to a deconfined phase with spontaneously broken Z_3 symmetry, where free gluons can exist [1]. The presence of dynamical quarks breaks the Z_3 symmetry of the Lagrangian. On the other hand, in the limit $m_q \rightarrow 0$ the QCD Lagrangian is characterized by exact chiral symmetry. Thus, in this limit one expects that, at high enough temperature, chiral symmetry will be restored (while spectroscopy tells us it must be broken in the zero-temperature, hadronic phase of QCD). For $n_f \geq 2$ this restoration may proceed by way of a first order transition [2], which could be expected to persist for small finite m_q . To check this phase diagram is not only of theoretical interest, but it may be relevant for the proposed heavy ion collision experiments and also has astrophysical consequences.

Numerical simulations of lattice QCD have become the prime tool for systematic first-principle checks of the validity of the above universality arguments [3]. In addition, numerical lattice studies can yield quantitative predictions about the value of the critical temperature and about the order of the transition. This has been demonstrated by the recent application of spectral density reweighting (SD) and finite-size scaling (FSS) techniques to the study of the deconfining phase transition in quarkless lattice SU(3) [4,5]. We consider it desirable to be able to apply the quantitative methods described in [5] to full QCD. This may be quite difficult in practice, since such methods tend to require large amounts of decorrelated data obtained at several temperatures on many lattices (including large ones).

In this letter, we report on an exploratory SD and FSS study of QCD with four quark flavors of mass $ma = 0.025$ (in lattice units). We ran on $L_t L^3$ lattices with $L_t = 4$ and $L = 6, 8, 10$. Our goal was to see what conclusions one could draw from such a limited experiment, using the methods described in [5]. We chose this particular combination of L_t , n_f and ma as a test case, since it has been previously studied by similar methods [6], and is unanimously believed to exhibit a first-order transition [6,7]. Beyond [6], we study not only the susceptibility of the Polyakov line, but also that of the chiral condensate and of the gluonic action density, as well as the partition function zeros. Like in [5], we use all these observables to estimate the infinite-volume critical coupling β_c , the latent heat, and the order parameter discontinuities.

Our simulations were performed using code developed by the MT_c group [8] to implement the Hybrid Monte Carlo [9] “ Φ algorithm” [10] for the full QCD action, defined in terms of the standard Wilson action for the SU(3) gauge fields and the Kogut-Susskind action for the fermion fields. The trajectory length was chosen to be 0.5; the acceptance was tuned to about 50% in the low-temperature (chiral symmetry broken) phase. (It is well-known [8] that the acceptance increases, for fixed simulation parameters, in the high-temperature, chirally symmetric phase. Thus, runs in the critical region show acceptances which vary between the $\approx 50\%$ characteristic of the hadronic phase, and $\approx 85\%$ seen in the chirally symmetric phase.)

For the reweighting analysis we kept measurements after each trajectory: for the average plaquette, the Polyakov loop and for the chiral condensate. (Note that one has to keep the measurements irrespective of whether the trajectory is accepted or rejected.) Reweighting allows us to reconstruct the β dependence in an appropriate small neighborhood $[\beta_{\min}, \beta_{\max}]$ around the coupling $\beta = \beta_0$ at which the simulation was run. Since reweighting is done in the gauge coupling β , only the gluonic (Wilson) action is used; the fermionic part of the action is absorbed into the density of states $\rho(S_p)$.

Our Monte Carlo (MC) calculations rely on 40000 measurements at $\beta_0 = 4.980$ for $L = 6$; 24000 measurements at $\beta_0 = 4.990$ for $L = 8$ and 20000 measurements at $\beta_0 = 4.992$ for $L = 10$. In figures 1, 2 and 3 we show for $L=6, 8$ and 10 the time history respectively for the average plaquette action S_p , Polyakov loop $Re(P)$ and the chiral condensate $\bar{\psi}\psi$. In each run, the first 2000 measurements were discarded for equilibration; for the remaining data the error bars were estimated using jackknife bins, corrected for bias using the double jackknife method [11].

In figure 4 we show the histograms for the probability density $f(S_p)$ for $L = 6, 8$ and 10. The probability density at a pseudo-critical coupling is expected to have a single or a double peak structure, according to the kind of phase transition it can represent. For $L = 6$ and 8 we see clear double peak structures as we would expect from figures 1 and 2, which feature “tunneling events” between “coexisting states” (the classic qualitative indication of a first-order transition). However for $L = 10$, $\beta_0 = 4.992$, we have not been able to see any such tunneling; correspondingly, the histogram is single-peaked. This means that these data cannot be included in our subsequent finite size scaling (FSS) fits. The recently proposed multicanonical algorithm [12] promises to help a lot in such situations. Unfortunately, the algorithm was not yet available when the present simulations were performed.

TABLE 1: Data reweighting range and partition function zeros.

L	β_0	$\beta_{\min}$	$\beta_{\max}$	S_{q_1}	S_{q_2}	β_x^0	β_y^0
6	4.980	4.9348	5.0149	0.444	0.504	4.9856(29)	0.0187(12)
8	4.990	4.9620	5.0166	0.450	0.505	4.9910(10)	0.0075(05)

In table 1 we show the reweighting validity ranges in β . These depend on which percentage of our action data obtained at β_0 we consider to give meaningful results when carrying out the extrapolation in β . As discussed in [5], we use q -tiles S_q of our gauge action to define this range:

$$\beta_{\min} = \beta_{q_1} \quad \text{and} \quad \beta_{\max} = \beta_{q_2} ,$$

where $q_1 = q$ and $q_2 = 1 - q$. The β_q can be found numerically by solving the implicit equation $S(\beta_q) = S_q$. The data in Table 1 are obtained using $q = 0.025$ (although this is quite small in view of our poor statistics, it does not make much difference in the final results).

Figure 1. Time history for the average plaquette for $L = 6, 8$ and 10 . We print the time evolution at every 20 trajectories for $L = 6$ and every 10 trajectories for $L = 8$ and 10 .

Within this range we proceed to calculate the partition function zeros, as well as the maxima of the specific heat and of the susceptibilities for the Polyakov loop and for the chiral condensate.

We refer to ref. [5] and its bibliography for a more detailed discussion of the partition function zero determination. Table 1 lists our estimates for the complex zeros (β_x^0, β_y^0).

Figure 2. Time history for the Polyakov loop $Re(p)$. We display the MC history as given in figure 1 caption.

For these lattices, the FSS fit of the imaginary part of u^0 , $u = e^{-\beta}$,

$$u_y^0(L) \sim L^{-1/\nu} \quad (1)$$

gives

$$\nu = 0.31 \pm 0.03, \quad (2)$$

for $L = 6$ and 8 . The inclusion of $L = 10$ may not be done as we have discussed above.

Figure 3. Time history for the chiral condensate $\bar{\psi}\psi$. Again we display the MC history as given in figure 1 caption.

It is remarkable how the infinite volume critical exponent ν , which for a first order transition is expected to be $\nu = 1/d = 1/3$, already seems to be obtainable from such small lattices. This resembles the situation for the SU(3) deconfining phase transition for $L_t = 2$ [5]. In that case we had obtained a consistent fit for ν already from $L = 6$ on.

Using the real parts of the zeros, $\beta_x^0(L)$, we can perform the fit

$$\beta_c^{\text{zeros}}(L) = \beta_c + \text{const } L^{-d}. \quad (3)$$

Figure 4. Histograms for the probability density $f(S_p)$ for our $L = 6, 8$ and 10 runs.

This yields our first estimate of the infinite volume critical coupling:

$$\beta_c^{\text{zeros}} = 4.9949 \pm 0.0027 . \quad (4)$$

To characterize the phase transition we also carry out a FSS analysis for the variance of the average plaquette action,

$$\sigma^2(S_p) = \langle S_p^2 \rangle - \langle S_p \rangle^2$$

The variance of the action is related to the specific heat by $C_v = \beta^{-2} \sigma^2(S_p)/V$, with $V = L^3$.

The large- L FSS behaviour distinguishes between first and second order transitions through the following fits

$$\sigma^2(S_p) = a_1 L^{\rho-d} + a_2 L^{-d} \quad \text{for a second order phase transition} \quad (5a)$$

and

$$\sigma^2(S_p) = a_1 + a_2 L^{-d} \quad \text{for a first order phase transition,} \quad (5b)$$

where $\rho = \frac{\alpha}{\nu}$. In this way the exponent ρ differentiates three interesting classes:

$$\begin{cases} 1. & \rho = 0 \quad \text{for noncritical behaviour,} \\ 2. & 0 < \rho < d \quad \text{for second order critical behaviour,} \\ 3. & \rho = d \quad \text{for a first order phase transition.} \end{cases} \quad (6)$$

The first order fit allows to determine the latent heat by the relation

$$\Delta s = 2\sqrt{a_1}. \quad (7)$$

A weak first order transition is a first order transition with a small latent heat. It is known to be numerically difficult to distinguish a weak first order from a strong second order transition, mainly when there is a lack of large lattice sizes and good statistics. The FSS scaling relations (5) are realized for the L dependent series of $\beta_{\max}(L)$ values defined by

$$\sigma^2(S_p; L) (\beta) = \text{maximum} \quad \text{for} \quad \beta = \beta_{\max}(L). \quad (8)$$

The corresponding maximum for the variances $\sigma_{\max}^2(s)$ and their respective couplings $\beta_{\max}$ are shown in table 2. No stable value for $\sigma_{\max}$ is obtained for $L = 10$ simulation within the validity β range. Again, this reflects the absence of tunneling in this run.

TABLE 2: Maximum and critical couplings for the plaquette variance $\sigma^2(s_p)$, Polyakov susceptibility $\chi(P)$ and for the chiral order parameter $\chi(C)$.

L	$10^4 \sigma_{\max}^2(s_p)$	$\beta_{\max}^s$	$10^3 \frac{\chi_{\max}(P)}{V}$	$\beta_{\max}^P$	$10^2 \frac{\chi_{\max}(C)}{V}$	$\beta_{\max}^C$
6	3.49(34)	4.9856(28)	4.24(34)	4.9870(26)	9.02(59)	4.9854(19)
8	3.47(32)	4.9913(01)	3.98(33)	4.9913(01)	7.82(57)	4.9912(13)

We make the hypothesis of a first order transition ($\rho = 3$) to fit our data to equation (5b) and our estimate of the latent heat is

$$\Delta s = (3.7 \pm 0.3) 10^{-2}. \quad (9)$$

Although the consistency of this fit can not be checked (the goodness-of-fit parameter cannot be computed since we only have two data points), the accuracy of the latent heat determination does give strong indications for a first order transition. Moreover,

a comparison of this value with our results for pure SU(3) [5] ($\Delta s = (3.09 \pm 0.05) 10^{-2}$ for $L_t = 2$, and $\Delta s = (3.16 \pm 0.06) 10^{-3}$ for $L_t = 4$) indicates that the first-order chiral phase transition in our four-flavor system is significantly stronger than in the pure gauge case for the same L_t . Like for the zeros, we again note the resemblance with $L_t = 2$ pure SU(3).

Next, we use the $\beta_{\max}(L)$ estimates of table 2 as input for the FSS fit (3) and our estimate of β_c is

$$\beta_c^{\text{specific heat}} = 4.9955 \pm 0.0021. \quad (10)$$

The FSS analysis for the maximum of the Polyakov loop susceptibility $\chi(P)$,

$$\frac{\chi(P)}{V} = \langle (ReP)^2 \rangle - \langle ReP \rangle^2 \quad (11)$$

and for the chiral condensate $\chi(C)$ is done in the same way.

In table 2 we show our reweighting results for $\chi_{\max}(P)/V$, $\chi_{\max}(C)/V$ and their corresponding couplings. Our FSS fits lead to the estimates

$$\beta_c^{\text{susc}} = 4.9944 \pm 0.0019. \quad (12)$$

$$\beta_c^{\text{chiral condensate}} = 4.9954 \pm 0.0026. \quad (13)$$

Although the accuracy for the critical couplings as obtained from different operators is not very restrictive, they are altogether consistent. Averaging over (4), (10), (12) and (13) and taking the smallest of the single error bars (all estimates rely on identical configurations and only differ due to systematic errors) we get

$$\beta_c = 4.99515 \pm 0.0019 \quad (14)$$

as our final estimate for the critical coupling.

In conclusion, even with rather limited statistics and relying only on fairly small-sized lattices, FSS and reweighting techniques are useful. At least the given estimates would provide much-needed help to determine appropriate parameters for further simulations on larger systems. The new algorithm [12] is expected to provide a sufficiently large number of tunneling events also for lattices with $L \geq 10$.

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