Thermodynamics and heavy quark potential in $N_f = 2$ dynamical QCD

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We study $N_f = 2$ lattice QCD with nonperturbatively improved Wilson fermions at finite temperature on $16^3 \times 8$ lattices. We determine the transition temperature at $m_\pi \sim 0.8$ and lattice spacing as small as $a \sim 0.12$ fm. The string breaking at $T < T_c$ is also studied. We find that the static potential can be fitted by a simple expression involving string model potential at finite temperature.

1. Introduction

Recent studies of $N_f = 2$ lattice QCD at finite temperature with improved actions have provided consistent estimates of $T_c$. Bielefeld group employed improved staggered fermions and improved gauge field action [1]. CP-PACS collaboration used improved Wilson fermions with mean field improved $c_{sw}$ and improved gauge field action [2]. Both groups were able to estimate $T_c$ in the chiral limit and their values are in a good agreement. Still there are many sources of systematic uncertainties and new computations of $T_c$ with different actions are useful as an additional check. We made first large scale simulations of the nonperturbatively $O(a)$ improved Wilson fermion action. Moreover we performed simulations with the lattice spacing $a$ much smaller than in studies by Bielefeld and CP-PACS groups. Our small lattice spacing helps us to determine parameters of the static potential in full lattice QCD at finite temperature. Our other goal is to study the vacuum structure of the full QCD at $T > 0$, in particular a relation between string breaking observed with the help of the Polyakov loop correlator at $T < T_c$ and abelian monopoles.

The fermionic action we employ is of the form

$$S_F = S_F^{(0)} - \frac{i}{2} g c_{sw} a^5 \sum_x \bar{\psi}(x) \sigma_{\mu\nu} F_{\mu\nu} \psi(x),$$

where $S_F^{(0)}$ is the original Wilson action, $c_{sw}$ is determined nonperturbatively [3]. We use Wilson gauge field action.

We took advantage of availability of $T = 0$ results obtained with the action [4] by UKQCD and QCDSF collaborations to fix the physical scale and $m_\pi / m_\rho$ ratio. Studies made by these collaborations also confirmed that $O(a)$ lattice artifacts are suppressed as expected [5]. We then may hope that lattice discretization errors of our results are small. So far only $N_t = 4$ and $6$ finite temperature results obtained with this action are available [6]. These results were obtained at rather large quark mass ($m_\pi / m_\rho > 0.85$) and lattice spacing.

Since $c_{sw}$ is only known nonperturbatively for $\beta \geq 5.2$, we have to work at rather large values of $\beta$. Thus to study transition at smaller values of the quark mass we need to go to larger $N_t$ values. This dictates our choice $N_t = 8$. We choose spatial extension of the lattice $N_s = 16$ as a compromise between computational burden and need to reduce finite size effects.
| $\kappa$ | # of traj. | $\kappa$ | # of traj. |
|--------|-----------|--------|-----------|
| 0.1330 | 3410      | 0.1330 | 1540      |
| 0.1335 | 1350      | 0.1335 | 1600      |
| 0.1340 | 2100      | 0.1337 | 12470     |
| 0.1343 | 2562      | 0.1340 | 10200     |
| 0.1344 | 3631      | 0.1345 | 1600      |
| 0.1345 | 3507      | 0.1345 | 1870      |
| 0.1346 | 350       | 0.1345 | 1870      |
| 0.1348 | 1515      | 0.1345 | 2650      |
| 0.1355 | 1801      | 0.1345 | 1870      |
| 0.1360 | 3699      | 0.1345 | 2650      |

Table 1. Simulation statistics.

It is known that in quenched QCD the order parameter of the finite temperature phase transition is Polyakov loop and corresponding symmetry is global $Z(3)$ symmetry. In chiral QCD the order parameter of the chiral symmetry breaking transition is the chiral condensate $\langle \bar{\psi} \psi \rangle$. There is no phase transition at intermediate values of the quark mass, only crossover. As numerical results show [1] both order parameters can be used to locate the transition point. We use only Polyakov loop leaving computation of the chiral condensate for future studies.

2. Simulation details

We use Hybrid Monte Carlo algorithm with parameters $\delta \tau = 0.0125$, $n_\tau = 20$, with acceptance rate about 70%. Simulations were done on Hitachi SR8000 at KEK and MVS 1000M at RAS, Moscow. We needed from 1000 ($\tau = 250$) to 3000 ($\tau = 750$) trajectories for thermalization, depending on $\kappa$ and $\beta$. Our simulations were performed for $\beta = 5.2, 5.25$. The values of $\kappa$ and corresponding number of trajectories are listed in Table 1.

We measured the Polyakov loop and plaqueette on every trajectory. They were used to measure corresponding susceptibilities. Depending on $\kappa$ every 5th, every 10th or every 20th trajectory were used to compute Polyakov loops correlator $\langle L_\vec{x} L_\vec{y} \rangle$, where $L_\vec{x} = $ Tr $P_\vec{x}$, $P_\vec{x} = \prod_{\vec{x}_0} U_{\vec{x}_0,\vec{x}_{0\vec{x}_{0}}}$. The MA gauge was also fixed on these configurations. Simulated annealing algorithm has been used to fix the gauge [8]. Abelian and monopole Polyakov loops, their susceptibilities and correlators were measured on gauge fixed configurations.

It turns out that for abelian and monopole observables the signal/noise ratio was better than that for gauge invariant nonabelian observables. This observation is in agreement with results from quenched QCD at $T > 0$ and both quenched and unquenched QCD at $T = 0$. For this reason we use abelian and monopole observables to determine transition temperature and to study string breaking. To obtain more precise results with our limited statistics we also employed hypercubic blocking introduced recently [9].

3. Transition temperature

In Fig[1] we show results for average of various kinds of Polyakov loops. One can see that $\langle L \rangle$ is a smooth function of $\kappa$. In the bottom part of this figure we show that as in quenched theory $\langle L_{Ab} \rangle \approx \langle L_{mon} \rangle / \langle L_{ph} \rangle$ and that $\langle L_{ph} \rangle$ does not show any changes at the transition. We determined $\kappa_1$, the critical $\kappa$, from the maximum
Figure 2. Nonabelian Polyakov loop susceptibilities (top), and abelian and monopole Polyakov loop susceptibilities at $\beta = 5.2$ (bottom).

of the Polyakov loop susceptibility. We found $\kappa_t = 0.1344(1)$ at $\beta = 5.2$ and $\kappa_t = 0.1340(1)$ at $\beta = 5.25$, see Fig. 2.

An interpolation formula for $r_0/a$ [4] gives us $T_c r_0 = 0.54(2)$ and $0.56(2)$. Or, using $r_0^{-1} = 394$ MeV, we obtain the critical temperature in physical units, $T_c = 213(10)$ and $220(5)$ MeV. Using again the data from [4] we get $m_\pi/m_\rho = 0.78, 0.82$ at the transition points. The susceptibilities for Abelian and monopole Polyakov loops have maxima at the same $\kappa$, see Fig. 2.

In Fig. 3 our results for transition temperature are shown in comparison with those of Refs. [1, 6]. Thus our results are in a good qualitative agreement with the results of the Bielefeld group.

4. String breaking

4.1. $T = 0$

At $T = 0$ string breaking has been observed so far with mixed operators including explicitly

static-light meson state and no sign of string breaking from Wilson loop has been found [10]. The last fact is believed to be due to very poor overlap of the broken string state with the Wilson loop operator. Keeping two terms in the Wilson loop spectral representation, corresponding to the string and two-meson states, one gets

$$W(r,t) = C_V(r) e^{-(V_0 + V_{str}(r)) t} + C_E(r) e^{-2E \cdot t},$$

where $V_{str}(r)$ is the usual confining potential and $E$ is the static-light meson energy. The overlap $C_V(r)$ is of $O(1)$ while $C_E(r)$ might be small. A quantitative estimate of this overlap has been suggested in [11] and then derived in abelian projection approach [12]: $C_E(r) \sim e^{-2E \cdot r}$. We believe that this is correct estimate at least in strong coupling, small $\kappa$ limit. If we assume that the real overlap is indeed of this order then the effect of the second term in eq. (2) would become detectable for both $r$ and $t$ of order of 2 fm, i.e. for very large Wilson loops with very small value. The real string breaking distance $r_{sb}$ is to be estimated from the equality of two exponents in eq. (2): $2m = \sigma \cdot r_{sb} - \pi/(12r_{sb})$, where $m = E - V_0/2$ may be called the string breaking energy or the effective quark mass [13]. The Wuppertal group result is $r_{sb} = 2.3r_0$ at $m_\pi/m_\rho = 0.7$ [13] and the CP-PACS result is $r_{sb} = 2.2r_0$ at $m_\pi/m_\rho = 0.6$ [11]. Taking the string tension in full QCD from Ref. [14], $\sqrt{\sigma} r_0 = 1.15(1)$, we get the effective quark mass $2m \sim 2.9/r_0 \sim 1.1$ GeV. This is in a surprisingly good agreement with estimate made in [13] using a different approach.
4.2. $T > 0$

At non-zero temperatures the string breaking has been observed in [13]. The heavy quark potential $V$ is related to the Polyakov loop correlator, $e^{-V(r,T)/T} = \langle L_\vec{z}L^\dagger_{\vec{y}} \rangle / 9$. In the limit $|\vec{x} - \vec{y}| \to \infty$, $\langle L_\vec{z}L^\dagger_{\vec{y}} \rangle$ approaches the cluster value $|\langle L \rangle|^2$, where $|\langle L \rangle|^2 \neq 0$ because the global $Z_3$ symmetry is broken by the fermions.

\begin{equation}
\langle L_\vec{z}L^\dagger_{\vec{y}} \rangle = \sum_{n=0}^{\infty} w_n e^{-E_n(r)/T},
\end{equation}

with integer $w_n$. At $T = 0$ we get $V(r,T) = E_0(r)$. In contrast, $V(r,T)$ at $T > 0$ gets contributions from all possible states. In pure gauge theory these are singlet and octet states and their excitations. Assuming that the excitations have much higher energies one can write

\begin{equation}
e^{-V(r,T)/T} = \frac{1}{9} e^{-V_{sing}(r,T)/T} \frac{8}{9} e^{-V_{oct}(r,T)/T}.
\end{equation}

In full QCD we must take into account the excited states. As it was discussed above in full QCD at $T = 0$ the singlet potential can be described by string model potential up to some distance $r_{br}$. Beyond this distance another state becomes the ground state of the system of two static quarks which one can call broken string state or two heavy-light mesons state. So there are two distinct states in the spectrum, one of which becomes the ground state at proper distance. The situation must be similar at small temperatures. We now assume that at temperatures $T < T_c$ the Polyakov loop correlator can be described with the help of these two states, namely string state and broken string (two meson) state. In this paper we do not single out the singlet potential. We understand that the contribution from the octet potential may contaminate our results. The work on calculation of the singlet and octet potential separately is in progress.

We now adopt the following representation for the Polyakov loop correlator

\begin{equation}
\frac{1}{9} \langle L_\vec{z}L^\dagger_{\vec{y}} \rangle = e^{-(V_0 + V_{str}(r,T))/T} + e^{-2E(T)/T},
\end{equation}

\begin{equation}
V_{str}(r,T) = -\left(\frac{\pi}{12} - \frac{1}{6} \arctan(2rT)\right) \frac{1}{r} + \frac{1}{2} \ln\left(1 + 4r^2T^2\right),
\end{equation}

\begin{equation}
E(T) = V_0/2 + m(T),
\end{equation}

where $m(T)$ is effective quark mass at finite temperature. The $T \neq 0$ string potential [13] was calculated in Ref. [17]. An alternative way to fit the static potential in full QCD at finite temperature was proposed long ago [18]:

\begin{equation}
V(r,T) = \frac{\hat{\sigma}}{\mu} (1 - e^{-\mu r}) - \frac{\alpha}{r} e^{-\mu r}
\end{equation}

with parameters $\hat{\sigma}$ and $\mu$. In [13] only $\mu$ [18] or only $\hat{\sigma}$ [19] are temperature dependent. We used function (6) to fit our data and compare with our model eq. (3)-(5).

Fig. 4 shows the nonabelian static potential for some values of $T/T_c$. The fit curves are two-state
5. Monopole Dynamics

We studied monopole density \( \rho \) and asymmetry in the monopole density \( \eta = (\rho_t - \rho_s)/(\rho_t + \rho_s) \) where \( \rho_t (\rho_s) \) is density of time-like (space-like) magnetic currents. In Fig. 6 we compare the monopole density in full and quenched QCD. Our results for quenched QCD were obtained on 16\(^3\)·8 lattice. The density in full QCD is substantially higher than that in quenched theory in agreement with previous studies.

\[
\frac{1}{g} \langle L_{\vec{x}} L_{\vec{y}} \rangle^{\text{mon}} = e^{-\langle V_{\text{str}}^{\text{mon}} (r,T) \rangle/T} e^{-2E_{\text{mon}}(T)/T} (7)
\]

\[
V_{\text{str}}^{\text{mon}} = \sigma_{\text{mon}} r \text{ and } E_{\text{mon}}(T) = V_0^{\text{mon}} + m_{\text{mon}}(T).
\]

The fit is shown in Fig. 4 by the solid line.
with our earlier results at $T = 0$ [20]. The behaviour of $\eta$ is qualitatively similar in both theories, i.e. $\eta$ is close to zero below transition and increases with temperature above $T_c$.

6. Conclusions and Outlook

Our results for $T_c$ obtained on $16^3 \times 8$ lattice at $\frac{\beta}{\kappa} \sim 0.8$ and lattice spacing small in comparison with work of Bielefeld group are in agreement with their results [1]. To test finite size effects and to determine transition temperature closer to the chiral limit we are planning to make simulations on $24^3 \times 8$ and $24^3 \times 10$ lattices.

Heavy quark potential has been measured in both phases. We introduced two-state parameterization eq.(3-5) for the heavy quark potential in confinement phase and found good agreement with numerical data obtained in that phase. Using this parameterization we computed string tension, quark effective mass and string breaking distance. We found that the ratio $\sigma(T)/\sigma(0)$ decreases toward the value 0.7 when $T$ approaches $T_c$. This value is substantially higher than the value obtained in quenched QCD. Whether this is due to systematic effects (meson-meson interaction, contribution of the octet potential, and some others) or is a physical effect deserves further study. Our results for the quark effective mass show good qualitative agreement with earlier results [3]. The results for string breaking distance imply that our fit might be inappropriate for temperatures $T/T_c > 0.95$.

We observed string breaking at $T < T_c$ also from abelian and monopole Polyakov loop correlators. We found that string tension, quark effective mass and string breaking distance calculated from the monopole Polyakov loops correlators are in agreement with the values obtained from the nonabelian correlators. Thus we found abelian and monopole dominance in the confinement phase of full QCD.

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