QCD at finite temperature and partially negative flavour numbers

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Abstract

We study dynamical fermion effects in lattice QCD at finite temperature. The method adopted is basically the extrapolation from negative flavour numbers already tested at zero temperature and based on the simulation of local bosonic theories, with an essential difference. With an appropriate choice of the boundary conditions on the bosonic fields, called “bermions”, it is possible to separate the $Z_3$ breaking contribution of fermion loops to the effective action from the one conserving $Z_3$: the former is simulated exactly at a fixed positive and even flavour number, while the extrapolation from negative flavour numbers is made only on the $Z_3$ invariant part of the action. We test this approach by comparing our results on a $16^3 \times 2$ lattice with those from a hopping parameter expansion and our results on a $16^3 \times 4$ lattice with those of direct Monte Carlo simulations including the fermion determinant.
1 Introduction

A new approach to the problem of estimating dynamical fermion effects in lattice QCD based on the extrapolation from theories with a negative number of dynamical flavours was recently proposed and applied in numerical simulations of the theory at zero temperature. In that case the quenched approximation appears to reproduce most of the experimental pattern of the hadronic spectrum and unquenching corrections are small when the comparison with the quenched case is performed after a suitable shift of the bare parameters i.e. at fixed values of the lattice spacing and of the renormalized quark mass. The “bermion” method exploits the smoothness of dynamical flavour dependence studied at fixed renormalized quantities to make estimates in full QCD which are extrapolations of results obtained at negative flavour numbers, where fermions are replaced by “bermions”, i.e. bosons with a fermion action [1, 2].

In this paper we extend this approach to QCD at finite temperature. The unquenching effects are not expected in this case to reduce to a simple renormalization with some small residual corrections. The SU(3) pure gauge theory is invariant under the discrete group $\mathbb{Z}_3$ and the deconfining transition in the theory is associated with the spontaneous breaking of this symmetry. In full QCD the $\mathbb{Z}_3$ symmetry is broken explicitly by fermion loops and the corresponding phase transition could disappear for intermediate values of quark masses. The straightforward application of the bermion method to finite temperature QCD would require an extrapolation from negative to positive flavour numbers $n_f$ also for the $\mathbb{Z}_3$ breaking fermion loop contribution to the effective action. This extrapolation seems quite unsafe because thermodynamical QCD observables, e.g. the critical temperature, are not expected to behave smoothly around $n_f = 0$. However it is possible, using appropriate boundary conditions on the bermion fields, to simulate theories where the $\mathbb{Z}_3$ breaking and the $\mathbb{Z}_3$ conserving contributions of fermion loops to the effective action get different weights corresponding to different “effective flavour numbers”. As a result, the $\mathbb{Z}_3$ breaking interaction can be simulated exactly for even and positive flavour numbers, while the $\mathbb{Z}_3$ conserving dynamical fermion contribution to the action, which is expected to give mainly a renormalization effect, is extrapolated from negative flavour numbers.

In section 2 we present the bermion action and the choice of the bound-
ary conditions which leads to the correct $Z_3$ breaking interaction. In section 3 we compare our results on a $16^3 \times 2$ lattice with those of a hopping parameter expansion [3] and our results on a $16^3 \times 4$ lattice with those of direct Monte Carlo simulations including the fermion determinant for $N_t = 4$ [4].

2 The role of the boundary conditions

The action for lattice QCD with $n_f$ flavours of Wilson fermion is

$$S[U, \psi, \bar{\psi}] = S_G[U] + \sum_{j=1}^{n_f} \sum_x \bar{\psi}_j(x) \gamma_5 [Q \psi_j](x)$$

(1)

where $S_G[U]$ is the gauge action, $j$ is a flavour index and $\gamma_5 Q$ is the Dirac operator:

$$[Q \psi_i](x) = \frac{1}{2\kappa} \gamma_5 \psi_i(x) - \frac{1}{2} \gamma_5 \sum_{\mu=0}^3 U_\mu(x)(1 - \gamma_\mu) \psi_i(x + \mu)$$

$$- \frac{1}{2} \gamma_5 \sum_{\mu=0}^3 U_\mu^+(x - \mu)(1 + \gamma_\mu) \psi_i(x - \mu)$$

(2)

After integration over the quark fields one obtains an effective action:

$$S_{eff}[U] = S_G[U] - n_f Tr(\log \gamma_5 Q)$$

(3)

where the second term is a sum of one loop diagrams. These can be divided into two classes: to the first belong the loops which lie entirely inside the lattice or wrap around the edges of the lattice a multiple of three times closing through the boundary conditions and to the second those which wrap a number of times different from multiples of three. At zero temperature all winding loops are just a finite volume effect, but at finite temperature, i.e. at finite physical extent of the “time” direction, the loops winding in this direction and belonging to the second class do influence the existence of the deconfining phase transition and an extrapolation from negative flavour numbers cannot be expected to be smooth. However, there are choices of the boundary conditions which affect only the second class and which reproduce the correct fermionic $Z_3$ breaking contribution also in the case where the fermion determinant is replaced by a bermion one.
The action for QCD with a negative flavour number $n_f$ is written in terms of $n_b = |n_f|/2$ bermions fields $\phi_j(x)$ which are commuting spinors:

$$S_b[U, \phi, \phi^\dagger] = S_G[U] + \sum_{x,y,z} \sum_{j=1}^{n_b} \phi^\dagger_j(x)Q(x, z)Q(z, y)\phi_j(y)$$  \hspace{1cm} (4)$$

where $j$ is a flavour index. We introduce a set of \textit{flavour dependent} boundary conditions parametrized by the elements of the center of the gauge group $Z_3$:

$$\phi_j(x, t + N_t) = -z_j\phi_j(x, t) \quad z_j \in Z_3$$  \hspace{1cm} (5)$$

The contribution of $n_b$ flavours to the second class of bermion loops in the effective action can be expressed as a sum of terms which are characterized by winding number modulo three $i$ of Polyakov loop-like terms $P_i$ in the “time” direction. The full expression for $S_{eff}$ can be parametrized as:

$$S_{eff} = S_G + n_b\text{Re}[P_0] + \text{Re}\left[\sum_{j=1}^{n_b} z_j P_1\right] + \text{Re}\left[\sum_{j=1}^{n_b} z_j^2 P_2\right]$$  \hspace{1cm} (6)$$

where $z_j$ is the element of $Z_3$ which fixes the boundary conditions of the $j$-th flavour. The property $z_j^3 = 1$ implies that the maximum power of $z_j$ that can appear in eq. (6) is two. The expression above should be compared with the corresponding fermion case with $n_f$ flavours and ordinary antiperiodic boundary conditions:

$$S_{eff} = S_G - \frac{n_f}{2}[\text{Re}(P_0) + \text{Re}(P_1) + \text{Re}(P_2)]$$  \hspace{1cm} (7)$$

The bermion boundary conditions can change the signs of $P_1$ and $P_2$ terms in the effective action: for example with two bermion flavours and the choice

$$z_1 = \exp(+2\pi i/3)$$
$$z_2 = \exp(-2\pi i/3)$$

one gets:

$$S_{eff} = S_G + 2\text{Re}(P_0) - \text{Re}(P_1) - \text{Re}(P_2)$$  \hspace{1cm} (8)$$

i.e. the contribution of two bermion flavours has been changed, for the second class of diagrams, into the one of two fermion flavours. We introduce a “normal” fermion number $n_f$ and two “magnetic” ones, $m_{f1}$ and $m_{f2}$ to
distinguish between loops with winding number 1 and 2 respectively and we write the effective action in the form:

\[ S_{\text{eff}} = S_G - \frac{n_f L}{2} \text{Re}(P_0) - \frac{m_{f1}}{2} \text{Re}(P_1) - \frac{m_{f2}}{2} \text{Re}(P_2) \] (9)

In table 1 we give, for various numbers of fermion flavours, the values of \( n_f, m_{f1} \) and \( m_{f2} \) that are obtained with specific choices of the boundary conditions. The correct fermion magnetic flavour numbers can be obtained only in some special cases. The extrapolations to positive \( n_f \) at fixed values of \( m_{f1} \) and \( m_{f2} \) can be made only for a few values: for example, for \( m_{f1} = m_{f2} = 2 \) the available \( n_f \) are \(-5\) and \(-2\). For the other cases the table includes a further choice of boundary conditions: the periodic ones (\( z_j = -1 \)). By adopting these conditions for some of the fermion flavours we can simulate theories where the values of \( m_{f1} \) and \( m_{f2} \) are different and also the contributions of terms with winding number larger than 2 are modified. In the case of moderately heavy quark masses where winding numbers higher than 2 can be neglected, the \( m_{f2} \) contributions can be seen as a small correction to the \( m_{f1} \) terms. In this case they can be extrapolated together with \( n_f \) terms. In the heavy quark mass case also the terms with winding numbers 2 can be neglected and the fate of \( m_{f2} \) terms ignored.

In the coming section we will investigate the role of the winding number 2 term: at \( N_T = 4 \) and for \( \kappa > 0.14 \) we find some evidence for the relevance of such a term.

3 Comparison with existing results

We have tested our method at \( N_t = 2 \) with the results of the hopping parameter expansion. According to ref. 3, the effective action in this approximation and at leading order reads:

\[ S_{\text{eff}} = S_G + H \sum_{\vec{x}} \text{Re} \text{Tr} \prod_{t=1}^{N_t} U_0(\vec{x}, t) + o(\kappa^4) \] (10)

where \( H = 2m_{f1}(2\kappa)^{N_t} \). The shift of the critical \( \beta \) value \( \beta_c(H) \) from \( \beta_c(0) \) can be predicted in term of the jumps of Polyakov loop and plaquette expectation values in the pure gauge theory:

\[ \beta_c(H) = \beta_c(0) - (4.94 \pm 0.75)H \] (11)
To leading order in $\kappa$ only terms with winding number 1 contribute and only the value of $m_{f1}$ is relevant. Periodic boundary conditions instead of antiperiodic ones are sufficient to promote bermion effects into fermion effects. In order to test the expression above, we have run different values of $n_f$ (from $-2$ to $-10$), $m_{f1}$ (from 2 to 6) and $\kappa$ (up to 0.071), while keeping the coefficient $8m_{f1}\kappa^2$ of the $Z_3$ breaking term in eq. 10 equal to a fixed value ranging from 0.01 to 0.08 and we have measured Polyakov loops and plaquettes. For this small values of $\kappa$ the effects of different values of $n_f$, which are of higher order in the hopping expansion, should be negligible and in fact the values of the observables at fixed $\beta$ depend only upon $8m_{f1}\kappa^2$. We have determined $\beta_c(H)$ by monitoring the jump in the Polyakov loop expectation value. The results, shown in fig. 1, are in remarkable agreement with the prediction of eq. 11, confirming the validity of the method in the hopping expansion regime.

Increasing $N_t$ and going to higher values of $\kappa$ represent a more severe test for the method. We have compared our results for $N_t = 4$ with those of hybrid Monte Carlo simulations of ref. [4], and in particular we have studied the behaviour of the Polyakov loops and of the plaquettes around the phase transition point. In this case the $m_{f1}$ term starts at the order $\kappa^4$, the renormalization effects due to “normal” fermion loops are not negligible anymore and we have to perform an extrapolation from negative values, at fixed values of $m_{f1}$. As already discussed, the values of $m_{f2}$ cannot be fixed at the fermionic ones at all values of $n_f$. In figures 2-4 we present the behaviour as a function of $\beta$ of the space-space plaquette $1-P_\sigma = \frac{1}{N_c}Re(Tr(U_1U_2U_3^1U_4^1))$ and of the absolute value of the Polyakov loop $L$, defined by:

$$L = \frac{1}{N_s} \sum_{\vec{x}} \frac{1}{N_c} Tr \prod_{t=1}^{N_t} U_0(\vec{x}, t)$$

(12)

for different values of $n_f$ and constant values of $m_{f1}$ at $\kappa = 0.12, 0.14$ and 0.16 respectively, together with the extrapolations to full QCD with two fermions ($n_f = m_{f1} = m_{f2} = 2$). In figures 5 we present for the case $\kappa = 0.14$ the results for the difference between space-space and space-time plaquettes.

The procedure adopted for the extrapolation is the following: we keep fixed the values of $\kappa$ and of a given observable ($P_\sigma$, $|P_\sigma - P_\tau|$ or $|L|$) and extrapolate the corresponding $\beta$ as a function of $n_f$. From previous applications of the bermion method to QCD at zero temperature it is known that, in
the intermediate quark mass region, a good extrapolation in $n_f$ is obtained by keeping fixed renormalized quantities. This is true in principle also for the simulations at finite temperature, however it must be noticed that our results refer, at least across the phase transition jump, to a rather heavy quark mass region where the renormalization effects are not so large to require a non perturbative treatment and therefore the extrapolation at fixed bare parameters gives a good first guess.

The results refer to the cases $a$, $b$, $c$ and $e$ of table 1 which correspond to $m_{f1} = 2$ and four different negative values of $n_f$. For small values of $\kappa$ the effect of the terms with winding number larger than one should be negligible and therefore, indipendently from the value of $m_{f2}$ the data should align as a function of $n_f$, as is the case for $\kappa = 0.12$ and 0.14. Even if they do not align we can consider two possible extrapolations which take into account the relevance of $m_{f2}$ terms. The first one is from the cases $b$ and $e$ where all the $Z_3$ breaking terms are fixed at the fermion value $m_{f1} = m_{f2} = 2$. The other one is to extrapolate from cases $a$ and $c$: it keeps fixed at the fermion value only the dominant $Z_3$ breaking term ($m_{f1} = 2$), while $m_{f2}$ is extrapolated from negative to positive values together with $n_f$. The results of the two extrapolations are given in the figures: they agree with each other and with the results of direct hybrid Monte Carlo simulations [4] showing the reliability of the method beyond the hopping expansion of eq. 10.

At $\kappa = 0.16$ we only show the full results for $n_b = 1, 2, 3$. The case $n_b = 2$ shows a different shape with respect to the other two and indicates the relevance of $m_{f2}$ terms. The simulations with $n_b = 5$ are only shown for the lowest values of $\beta$. We have observed that in this case the correlation times increase by almost two order of magnitude showing a severe critical slowing down. This may be ascribed to the delicate cancellation of “magnetic” effects among three out the five fermion flavours. We plan to further study algorithms to improve the thermalization in a multiboson environment. In the region where we can perform the separate extrapolations of $n_b = 1, 3$ and $n_b = 2, 5$ results we observe again a reasonable consistency among them.

We have shown that, by suitably modifying the boundary conditions, the fermion method can be applied to the study of full QCD at finite temperature and compared successfully with existing results. A detailed analysis of the nature of the phase transition, of the form of the effective action and of the possible interruption of the phase transition line for lower values of quark masses is currently under study [5].
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Table 1: The effective flavour numbers $n_f$, $m_{f1}$ and $m_{f2}$ obtained with boundary conditions $z_j$ in theories with $n_b$ bermion fields.

| case | $n_b$ | $z_j$ | $n_f$ | $m_{f1}$ | $m_{f2}$ |
|------|-------|-------|-------|----------|----------|
| a    | 1     | $z_1 = -1$ | -2    | 2        | -2       |
|      | b     | $z_1 = e^{\frac{2\pi i}{3}}$ | $z_2 = e^{-\frac{2\pi i}{3}}$ | -4    | 2        | 2        |
| c    | 3     | $z_1 = z_2 = -1$ | $z_3 = 1$ | -6    | 2        | -6       |
| d    | 4     | $z_1 = e^{\frac{2\pi i}{3}}$ | $z_2 = e^{-\frac{2\pi i}{3}}$ | $z_3 = 1$ | $z_4 = -1$ | -8    | 2        | -2       |
|      | e     | $z_1 = z_2 = e^{\frac{4\pi i}{3}}$ | $z_3 = z_4 = e^{-\frac{2\pi i}{3}}$ | $z_5 = 1$ | -10    | 2        | 2        |
|      | f     | $z_1 = -1$ | $z_2 = 1$ | -4    | 0        | -4       |
|      | g     | $z_1 = e^{\frac{2\pi i}{3}}$ | $z_2 = e^{-\frac{2\pi i}{3}}$ | $z_3 = 1$ | -6    | 0        | 0        |
|      | h     | $z_1 = z_2 = -1$ | $z_3 = z_4 = 1$ | -8    | 0        | -8       |
|      | i     | $z_1 = e^{\frac{2\pi i}{3}}$ | $z_2 = e^{-\frac{2\pi i}{3}}$ | $z_3 = z_4 = 1$ | $z_5 = -1$ | -10    | 0        | -4       |
|      | l     | $z_j = -1$ ($j=1,\ldots,n$) | $n$ | $-2n$    | $2n$    | $-2n$    |
Figure 1: The critical value of $\beta$ in bermion simulations on a $16^3 \times 2$ lattice as a function of $8m_{f1}\kappa^2$ is compared with the hopping expansion prediction [2] (see eq. 11).
Figure 2: The average space-space plaquette $1 - P_\sigma$ and the absolute value of the Polyakov loop $|L|$ on a $16^3 \times 4$ lattice for $\kappa = 0.12$ for four simulations with negative $n_f$ (corresponding, from right to left, to cases $e$, $c$, $b$, $a$ of table 1) and the extrapolations to the fermion case $n_f = 2$ discussed in the text ($\star$: extrapolation from cases $a$ and $c$; $\times$: extrapolation from cases $b$ and $e$).
Figure 3: The same as in fig. 2 for $\kappa = 0.14$. 
Figure 4: The same as in fig. 2 for $\kappa = 0.16$. 

\[ 1 - P_{\sigma} \] 

\[ |L| \] 

$\beta$
Figure 5: The difference between space-space and space-time plaquettes for $\kappa = 0.14$ for four simulations with negative $n_f$ (corresponding, from right to left, to cases $e$, $c$, $b$, $a$ of table 1) and the extrapolations to the fermion case $n_f = 2$ discussed in the text ($\ast$: extrapolation from cases $a$ and $c$; $\times$: extrapolation from cases $b$ and $e$).