First Order Phase Transition in Finite Density QCD using the modulus of the Dirac Determinant.

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ABSTRACT

We report results of simulations of strong coupling, finite density QCD obtained within a MFA inspired approach where the fermion determinant in the integration measure is replaced by its absolute value. Contrary to the standard wisdom, we show that within this approach a clear signal for a first order phase transition appears with a critical chemical potential in extremely good agreement with the results obtained with the Glasgow algorithm. The modulus of the fermion determinant seems therefore to preserve some of the relevant physical properties of the system. We also analyze the dependence of our results on the quark mass, including both the chiral and large mass limit, and the theory in the quenched approximation.
Non-perturbative investigations of QCD at finite temperature and density have received much attention in the last years. The aim of these investigations is to find the matter conditions in the early Universe and to get a clear insight into experimental signatures in the heavy-ion collision experiments. Even if considerable progress has been achieved in the investigations of QCD at finite temperature and zero chemical potential using the lattice approach, the present situation of the field at finite density is not so satisfactory. As is well known, the complex nature of the determinant of the Dirac operator at finite chemical potential, which makes it impossible to use standard simulation algorithms based on positive-definite probability distribution functions, has much delayed investigations on the full theory with dynamical fermions. On the other hand the quenched approximation, which has been extensively and successfully used in simulations of QCD at zero chemical potential, seems to have some pathological behaviour when applied to QCD at finite density.

We discuss in this paper some features connected to simulations in finite density QCD. The main topic concerns the use of the absolute value of the fermionic determinant. We show that, against some theoretical prejudices based on random matrix models, the relevant physical features of finite density QCD seem to be preserved after taking the absolute value of the Dirac-Kogut-Susskind operator.

As well known, the partition function of finite density QCD

$$Z = \int [dU] e^{-\beta S_G(U)} \det \Delta(U, m, \mu).$$

(1)

can be written as the product of the following two contributions

$$Z = \langle e^{i\phi_{\Delta}} \rangle \left[ \int [dU] e^{-\beta S_G(U)} |\det \Delta(U, m, \mu)| \right].$$

(2)

where the first factor in (2)

$$\langle e^{i\phi_{\Delta}} \rangle = \frac{\int [dU] e^{-\beta S_G(U)} e^{i\phi_{\Delta}} |\det \Delta(U, m, \mu)|}{\int [dU] e^{-\beta S_G(U)} |\det \Delta(U, m, \mu)|}$$

(3)

accounts for the mean value of the cosine of the phase of the fermion determinant computed with the probability distribution function of the pure gauge theory times the modulus of the fermion determinant. The second factor of (2) is just the partition function we will use along this work. The first factor in (2) gives a net contribution to the free energy density only in the case in which it falls off exponentially with the lattice volume. For random matrix models it has been shown that this is what happens and this is the origin.
for the theoretical prejudices about the relevance of the phase in QCD. Early simulations of QCD with the absolute value of the fermion determinant in small lattices \[4\] seem to corroborate these theoretical prejudices.

For the abelian model in 0+1 dimensions it can be shown also that the first factor of (2) plays a fundamental role \[5\] and this is also the case for four dimensional QED as follows from the fact that the abelian model shows no dependence on the chemical potential \(\mu\) or in other words, from the absence of baryons in this model. Notwithstanding that, it can be shown that the phase of the determinant is completely irrelevant in 0+1 dimensional QCD \[6\] but unfortunately no analytical results on this subject are available for four dimensional QCD.

In order to check to what extent taking the absolute value of the fermion determinant in the integration measure is a good approximation for full QCD at finite baryon density, we report here results for the number density as a function of the chemical potential \(\mu\) at infinite gauge coupling, where more data are available in the literature \[7\], \[8\]. The results for larger \(\beta\), in particular in the physically interesting scaling region, will be presented elsewhere.

Our numerical simulations have been performed using a MFA \[9\] inspired approach. The idea is to consider \(\det \Delta\) or its absolute value as an observable. In this case \(\det \Delta\) is not in the integration measure, and one avoids the problem of dealing with a complex quantity in the generation of configurations. This can be done in a (in principle) exact way by means of the MFA algorithm \[9\] where the mean value of the determinant at fixed pure gauge energy is used to reconstruct an effective fermionic action as a function of the pure gauge energy only. Up to now this method has been successfully used in several models (at zero density), where it allows free mobility in the \(\beta - m_q\) plane, including the chiral limit \[9\].

We used the GCPF (Grand Canonical Partition Function) formalism to write the fermionic determinant as a polynomial in the fugacity \(z = e^{\mu}\) \[10\]:

\[
\det \Delta(U; m_q, \mu) = \det \left( G + e^{\mu}T + e^{-\mu}T^\dagger \right) = z^{3V} \det \left( P(U; m_q) - z^{-1} \right)
\]

\[
= \sum_{n=-3L_t^3}^{3L_t^3} a_n z^{nL_t} \tag{4}
\]

where the propagator matrix is

\[
P(U; m_q) = \begin{pmatrix} -GT & T \\ -T & 0 \end{pmatrix}
\]
in which $G$ contains the spatial links and the mass term, $T$ contains the forward temporal links and $V$ is the lattice volume. Once fixed $m_q$, a complete diagonalization of the $P$ matrix allows to reconstruct $\det \Delta$ for any $\mu$. Due to the $Z(L_t)$ symmetry of the eigenvalues of $P$ it is possible to write $P^{L_t}$ in a block matrix form and we only need to diagonalize a $(6L_s^3 \times 6L_s^3)$ matrix; the chiral limit is straightforward since it only consists in diagonalizing $P(U; m_q = 0)$.

Alternatively, one could directly diagonalize the fermionic matrix, expressing the determinant as a polynomial in the mass. In this way one is allowed to freely move in the fermionic mass, and this can be useful for the determination of chiral observables, but simulations have to be repeated for each value of the chemical potential. Also, this method tends to be more computer demanding, since it requires the diagonalization of larger matrices.

The partition function (1) is real, and positive definite; in particular, the average fermionic determinant at fixed energy is positive definite. This is no longer the case even in large but finite statistics: while the average determinant can be made real, its sign is not definite. Therefore, and according to the previous discussion, we have chosen to compute $Z$ by taking the absolute value of the fermionic determinant on a configuration by configuration basis. With the available statistics also other definitions we used to obtain a positive definite partition function (like the modulus of the averaged coefficients or the modulus of the real part of the coefficients, instead of the average of the modulus) gives results that can not be distinguished among them and with the previous definition.

We have performed simulations in $4^4$, $6^3 \times 4$ and $8^3 \times 4$ lattices, at $\beta = 0$ with various values of fermion masses, starting from $m_q = 0$. The analysis we report in this letter only concerns the behaviour of the baryonic number density $N(\mu)$ and that of its derivative with respect to $\mu$, which in the thermodynamical limit is proportional to the radial density of the zeros of the partition function. A more comprehensive analysis, reporting in particular the behaviour of chiral parameters is under way and will be published elsewhere.

The results for $\beta = 0$, $m_q = 0.1$, in $4^4$ and $6^3 \times 4$ lattices are reported in Figs. 1, 2. The values of the parameters have been chosen to allow a direct comparison with 2, 3. Several comments are in order

1. In the smaller volume, neither $N(\mu)$ nor the radial density indicate a critical behaviour, apart from the (unphysical) behaviour near the onset threshold $\mu_o = 0.31$. The small $\mu$ behaviour is unchanged in the larger volume, but a structure develops at $\mu_c = 0.69$ as well as $\mu_s \simeq 0.96$,
which indicates a phase transition in the same position as that found by Karsch et al. [8] as well as a (first order) saturation transition, for which we lack of physical explanations. This contradicts the hypothesis [11] that taking the modulus of the determinant washes out the transition.

2. Our results are in very good agreement with others obtained with different methods. In particular, up to $\mu_c$ we are in striking agreement with Barbour et al. [7], reproducing both the "unphysical" behaviour at small $\mu$ and the transition at $\mu_c$. The value of $\mu_c$ agrees with that obtained in [8], but our discontinuity is steeper, corresponding to a higher peak in the radial distribution of zeros (see Fig. 2).

3. The value $\mu_o$ at which $N(\mu)$ departs from zero coincides with that found in [8]. Contrary to $\mu_c$, however, the peak at $\mu_o$ of the radial density of zeros does not drastically increase with the volume, as expected for a critical behaviour. We tend to exclude a first order phase transition at $\mu_o$.

4. The saturation at $N(\mu) = 1$ is not reached smoothly in the larger volumes, indicating a transition at $\mu_s \approx 0.96$. Also the radial density of zeros reported in [7] shows a peak consistent with the existence of this transition.

The behaviour sketched above permains for values of fermion mass as low as 0.02. At lower masses the behaviour of the observables becomes smooth in $4^4$ and $6^3 \times 4$ lattices. In Fig. 3 we report preliminary results of a simulation at $m_q = 0, \beta = 0$ in a $8^3 \times 4$ for the radial density of the zeros superimposed with the same data for the smaller lattices. In this lattice a clear signal of transition develops at $\mu_c = 0.65$ as well as near saturation. This behaviour strongly suggests that the claim [11], that taking the modulus of the fermion determinant destroys the transition, is unjustified and what is observed is indeed a volume effect, as function of the fermionic mass, disappearing consistently in larger lattices. It is interesting to notice that (although more statistics is needed) the value of $\mu_c$ here obtained agrees with the chiral limit extrapolation of the value obtained in [8].

In Fig. 4 we report the dependence of $\mu_o$, $\mu_c$ and $\mu_s$ on the quark mass. One could expect that the partition function computed with the modulus of the determinant contains in the spectrum meson states with non zero baryonic charge, as in a theory with adjoint fermions in addition to usual ones. In this case one could expect a link between the features in $N(\mu)$ and the mass of the lightest of such states, degenerated with the ordinary pion.
In the figure we also plot the strong coupling/mean field value of half the mass of the pion. Looking at the figure we can see that the onset $\mu_o$ follows rather closely the pion mass, at least for $m_q < 0.3$; for larger values of $m_q$ a clear displacement can be seen. Moreover the exact values of $\mu_o$ are better described, in the former region, by a simpler relation, i.e. the square root of the quark mass. If colourless diquark states, with non zero baryonic charge, lighter than the nucleon exist we would expect a saturation transition as soon as the chemical potential is of the order of magnitude of (half) the mass of the particle. Our data for $N(\mu)$ seem to discard this scenario; the (almost) linear behaviour between onset and the transition is not modified in the largest lattice.

We have also considered the quenched case where no signals of transition have been found. In this case we compute the derivative of $N(\mu)$, which is given by the distribution of the eigenvalues of the propagator matrix, and shows no sharp peaks for any $\mu$ ($6^3 \times 4$). The distribution is reported in Fig. 5, superimposed with that of the full theory; the inclusion of dynamical fermions is therefore crucial for the revealing of the transition.

In the full theory at large masses we have found results inconsistent with expectations. The signal of the phase transition vanishes for $m_q > 0.7$ and $N(\mu)$ goes smoothly from zero to one except for two structures at the onset and saturation point; this is consistent with what reported in [7].

To understand the results for large masses, we performed simulations in the smaller lattice ($4^4$) diagonalizing directly the $\Delta(m_q = 0)$ matrix for several values of $\mu$. This way $Z$ can be computed (essentially) continuously in the mass. The results in the small mass range are consistent with the ones obtained from the eigenvalues of the propagator matrix, i.e. no transition is found in the same lattice. At larger values of mass, instead, a clear transition signal appears and, as expected on phenomenological grounds, it shows a saturation behaviour at a value of the chemical potential consistent with the large mass extrapolation of the results of [8]. This is shown in Fig. 6 for $m_q = 1.5$; in the same figure we also report preliminary results for the chiral condensate.

In conclusion, the situation is still far from clear. We have shown that using the modulus of the determinant we can reproduce the results obtained with other algorithms and this is the main motivation of this letter. However, the behaviour from the onset to the transition at $\mu_c$ is difficult to understand in physical terms, as is the significance of the onset; we expect to get more informations from the analysis of chiral observables that we will present in a future publication. For large masses the technique based on the propagator
matrix seems to suffer from numerical instabilities which may wash out the transition signal. On the other hand, the simulations performed diagonalizing directly the fermionic matrix appear to give results in agreement with physical intuition.

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Figure 1: Number density vs. chemical potential in a $4^4$ (dots) and $6^3 \times 4$ (diamonds) lattice at $m_q = 0.1$
Figure 2: Radial density of zeros in a $4^4$ (dots) and $6^3 \times 4$ (continuous line) lattices at $m_q = 0.1$
Figure 3: Radial density of zeros in a $4^4$ (dots), $6^3 \times 4$ (continuous line) and $8^3 \times 4$ (histogram) lattices at $m_q = 0.0$
Figure 4: $\mu_o, \mu_c$ and $\mu_s$ in the $(\mu, m_q)$ plane in a $6^3 \times 4$ lattice
Figure 5: Radial density of zeros quenched (histogram) and unquenched (continuous line) in a $6^3 \times 4$ lattice at $m_q = 0.1$. 
Figure 6: Number density (squares) and chiral condensate (diamonds) vs. chemical potential in a $4^4$ lattice at $m_q = 1.5$. The arrow indicates the transition point obtained from an extrapolation of the data in [8].