Lattice simulations of QCD with $\mu_B \neq 0$ versus phase quenched QCD

K. Splittorff

1 Nordita, Blegdamsvæj 17, DK-2100, Copenhagen Ø, Denmark

(Dated: November 20, 2018)

Previously published lattice results for QCD at $\mu_B \neq 0$ are compared to analytic predictions for phase quenched QCD. We observe that the strength of the sign problem in QCD is linked directly to the position of the phase transition line for pion condensation in phase quenched QCD and that the number of terms needed in the Taylor expansion approach depends on the strength of the sign problem. Together this emphasizes the physical importance of the sign problem and helps to clarify the range over which the Taylor expansion approach is practically applicable. Finally, we observe that the positions of the endpoint of the first order chiral phase transition in the QCD phase diagram found in two successive computations by Fodor and Katz are both close to the position of the phase transition line for pion condensation in phase quenched QCD.

INTRODUCTION

Results from lattice simulations for unquenched QCD at non-zero baryon chemical potential give us valuable information about the non-perturbative sector of strongly interacting matter. The central aim of the lattice simulations at non-zero baryon chemical potential is to determine the phase diagram of unquenched QCD. The focus at present is on the chiral transition as a function of temperature and rather small chemical potential. Predictions for the slope of the chiral crossover line at zero chemical potential and for the position of the endpoint of the first order chiral phase transition have already been set forth. Lattice simulations at zero-baryon chemical potential are, however, different from lattice simulations at zero baryon chemical potential in that they have to deal with the sign problem. The term ‘sign problem’ is used to describe the numerical difficulties in doing Monte Carlo sampling on a non-positive weight. The presence of the sign problem is a direct consequence of the imbalance between quarks and anti-quarks one imposes in order to generate a non-zero baryon density. Moreover, the sign problem has several direct physical implications. One of the most dramatic can be seen if we compare to phase quenched QCD.

Phase quenched QCD is different from QCD in that one takes the absolute value of the fermion determinant in the measure

$$Z_{PQ} = \int [dA_\eta] \det(D_\eta \gamma_0 + \mu \gamma_0 + m)^{N_f} e^{-SYM}. \quad (1)$$

The phase diagram of this theory has an extended region which is dominated by a Bose-Einstein condensate of pions. Returning to QCD by including the phase of the determinant wipes out this pion phase entirely. In order to deal with the phase of the determinant in lattice simulations of QCD three main approaches have been pursued: 1) the Taylor expansion approach [1, 2, 3, 4, 5], 2) the reweighting approach [6, 7, 8, 9, 10], and 3) the imaginary chemical potential approach [11, 12].

In this paper we address some of the issues involved in the interpretation of existing lattice data for QCD at non-zero baryon chemical potential obtained with these approaches. We will do so by comparing previously published lattice data for QCD at non-zero baryon chemical potential to phase quenched QCD. First of all we replot a lattice measurement from [5] of the variance of the phase of the determinant in units where we can compare to analytic predictions for phase quenched QCD. We observe that the contour lines for the variance of the phase of the determinant are aligned with the phase transition line for pion condensation in phase quenched QCD. Moreover, the distance between the contour lines decreases as the values of $\mu$ and $T$ approach the region where phase quenched QCD is in the pion phase. Next, we wish to verify, as stated in [4], that the order of the Taylor expansion needed depends on the strength of the sign problem. In order to do so we consider the 6th order Taylor expansion of the quark number susceptibility published in [5]. In agreement with the statement of [4] we find that the 6th order term in the expansion becomes important when the variance of the phase exceeds a certain value. Together with the first observation we conclude that it will be exceedingly hard to make predictions for QCD at non-zero baryon chemical potential using the Taylor expansion approach when the values of $\mu$ and $T$ are such that pion condensation occurs in phase quenched QCD.

Finally, we consider the values of $\mu$ and $T$ at the endpoint of the first order chiral phase transition as found using the reweighting method in [6] and [8]. After rescaling the coordinates for the endpoint we observe that both predictions occur at values of $\mu$ and $T$ which are close to the phase boundary for pion condensation in phase quenched QCD.

PIION CONDENSATION IN PHASE QUENCHED QCD

At zero temperature the critical chemical potential for pion condensation in phase quenched QCD is $\mu = m_\pi/2$ and at small temperature the critical chemical potential
can be evaluated in chiral perturbation theory \[13\]. The critical temperature found at 1-loop order corresponds to the semi-classical result for the critical temperature of Bose-Einstein condensation in a dilute massive Bose gas. The general determination of this phase transition can be evaluated directly by means of Monte Carlo simulations of phase quenched QCD and such studies are currently taking place \[14\]. One can also estimate the position of the phase transition using phenomenological models. Probably the simplest prediction for the critical temperature in phase quenched QCD is obtained from the random matrix model considered in \[13\]. This mean field approach leads to a critical temperature (see eq (5.48) of \[13\]) which depends both on the chemical potential, the quark mass and the phenomenological constant introduced in the model. However, by taking the quark mass to zero while keeping the ratio of the pion mass to the chemical potential fixed the dimensional constant drops out and the result for the critical temperature \[T_c\] in phase quenched QCD is (\(T_0\) is the pseudo critical temperature for chiral symmetry breaking at \(\mu = 0\))

\[
T_c/T_0 = \sqrt{1 - \left(\frac{m_\pi}{2\mu}\right)^4}.
\]

(2)

In the range \(m_\pi/2 < \mu < m_\pi\) this simple result agrees well with the predictions from the NJL model \[16\] \[17\], the prediction from strong coupling QCD \[18\], as well as the predictions from a random matrix model with all Matsubara frequencies included \[17\]. At larger values of the chemical potential the critical temperature obtained in these models drops down to zero again as a result of saturation.

The \(\mu\) dependence of the critical temperature given in \(2\) is also consistent with the picture emerging from the lattice studies of phase quenched QCD \[14\]. These lattice simulations and analytical arguments \[13\] \[14\] however suggest that the order of the pion phase transition changes from 2nd order to 1st order with increasing chemical potential. This aspect is not reproduced by the random matrix model.

THE VARIANCE OF THE PHASE

A direct measure of the sign problem in QCD is the variance of the phase, \(\theta\), of the fermion determinant. The phase was measured in \[3\] \[21\] and a contour diagram with lines of constant variance, \(\sqrt{\langle \theta^2 \rangle - \langle \theta \rangle^2}\), in the \((T/T_0, \mu/T)\)-plane was given. Below we replot the data from \[3\] as a contour diagram in the \((2\mu/m_\pi, T/T_0)\)-plane, \(T_0\) again being the pseudo-critical temperature for the crossover at \(\mu = 0\). The value of the pion mass used in order to convert the plot from \[3\] is \(m_\pi/T_0 = 3.58\). Shown are contour lines for \(\sqrt{\langle \theta^2 \rangle - \langle \theta \rangle^2} = \pi/4, \pi/2, 3\pi/4, \ldots, 2\pi\), the values increasing with the chemical potential. Note that contour lines for \(\sqrt{\langle \theta^2 \rangle - \langle \theta \rangle^2} > 2\pi\) are not displayed. In addition to the contour lines the prediction \(2\) for the critical temperature for pion condensation in phase quenched QCD is shown. The contour lines are seen to be aligned with the phase transition line and the distance between the contour lines decreases as the phase transition line is approached. This observation is consistent with the fact that the presence of the phase of the determinant wipes out the pion phase transition. In particular, it is natural to expect that \(\sqrt{\langle \theta^2 \rangle - \langle \theta \rangle^2} \gg 1\) in the region where phase quenched QCD enters the pion phase, even with a moderate volume. At zero temperature this has been verified analytically \[21\] \[22\]: the eigenvalue density of the Dirac operator in QCD with \(\mu \neq 0\) becomes highly oscillating for \(\mu > m_\pi/2\) and it is these oscillations which insure that the pion phase is avoided in QCD \[23\]. Note that the contour lines shown in figure\(1\) will shift toward lower values of \(\mu\) and higher values of \(T\) with increasing volume (for a discussion of the volume dependence of the variance see \[20\]).

TAYLOR EXPANSIONS

One of the approaches to QCD at non-zero quark number chemical potential which are being pursued \[2\] \[4\] \[5\] is based on a Taylor expansion in \(\mu/T\) around \(\mu = 0\).
First, the forms of the traces contributing to an operator at a given order in the chemical potential are determined analytically and then these traces are evaluated by standard Monte Carlo methods at $\mu = 0$. Traces contributing to order $2n$ in the Taylor expansion of an extensive observable are typically of order $V^n$ and these terms must combine to a result linear in the volume $V$. This makes it difficult to control numerical errors in a high order expansion.

In the Taylor expansion depends on the severity of the sign problem. Here we verify this statement using the quark number susceptibility determined in [5] to 6th order in the chemical potential. Here we verify this statement using the quark number susceptibility determined in [5] to 6th order in the chemical potential. For the three largest values of $\mu/T$ the result from the 4th order Taylor expansion are indicated by the dashed lines. From this plot we estimate the values of $T/T_0$ below which the 6th order term in the Taylor expansion of the quark number susceptibility becomes important.

In figure 2 it is stated that the order of terms needed in the Taylor expansion depends on the severity of the sign problem. Here we verify this statement using the quark number susceptibility determined in [5] to 6th order in the chemical potential. For the values of $\mu/T$ given in figure 2 for $\mu/T = 0.0, 0.8, 1.0$, we observe that the 6th order term in the Taylor expansion depends on the severity of the sign problem. Here we verify this statement using the quark number susceptibility determined in [5] to 6th order in the chemical potential. For the three largest values of $\mu/T$ the result from the 4th order Taylor expansion are indicated by the dashed lines. From this plot we estimate the values of $T/T_0$ below which the 6th order term in the Taylor expansion of the quark number susceptibility becomes important. These values are indicated by the three crosses in figure 3. We observe that the 6th order term in the determination of the quark number susceptibility becomes important for values of $\mu$ and $T$ where the variance of the phase is larger than $\pi/4$. That is, the 4th order Taylor expansion of the quark number susceptibility in [5] is only appropriate to the left of the leftmost contour line in figure 2. Given the sufficient numerical accuracy to handle the delicate cancellations of the terms of order $V^6$, the 6th order Taylor expansion of the quark number susceptibility approach may be adequate somewhat to the right of the $\sqrt{\langle \theta^2 \rangle - \langle \theta \rangle^2} = \pi/4$ contour line.

Combined with the observations made from figure 2 we conclude that even for small volumes it will be extremely difficult to make predictions for observables in QCD using the Taylor expansion approach when the values of $\mu$ and $T$ are such that phase quenched QCD is in the pion phase.

Certainly, our estimate above only serves as a first numerical test of the proposition that the number of terms needed in the Taylor expansion depends on the severity of the sign problem. A dedicated series of measurements of several observables on the lattice are needed in order to settle this firmly.

**CRITICAL ENDPOINT**

In this section we compare the positions of the endpoints of the first order chiral phase transition as determined in [5] and [8] to the estimated position of the pion phase.
phase transition in the phase quenched theory\(^1\). In order to facilitate this comparison we again consider the plane \(2\mu/m_\pi, T/T_0\) and plot in figure 4 simultaneously the critical endpoints determined for QCD in \(\text{[8]}\) and \(\text{[9]}\) and the position of the pion phase transition for phase quenched QCD given in \(\text{[2]}\). The values of the pion mass used in order to make the rescaling was \(m_\pi = 294\text{MeV}\) for \(\text{[8]}\) and \(m_\pi = 145\text{MeV}\) for \(\text{[9]}\).

We observe that the endpoints found in \(\text{[8]}\) and \(\text{[9]}\) both are remarkably close to the phase transition line estimated in \(\text{[2]}\) for phase quenched QCD. (The fact that the chemical potential at the endpoint scales with \(m_\pi\) was noted in \(\text{[4]}\).)

The phase transition into the pion phase occurring in phase quenched QCD has a very simple manifestation in the eigenvalue spectrum of the Dirac operator: it occurs when the density of eigenvalues of the Dirac operator reaches the quark mass (see e.g. \(\text{[24]}\) or \(\text{[22, 25]}\)). That is, the critical chemical potential and temperature are determined by

\[ \rho_{\text{PQ}}(z = m, m, T, \mu) \neq 0, \]  
(3)

where the eigenvalues are given by

\[ (D_\eta \gamma_0 + \mu \gamma_0)\psi_n = z_n \psi_n \]  
(4)

and the eigenvalue density is

\[ \rho_{\text{PQ}}(z, m, T, \mu) = \left( \frac{1}{V} \sum_n \delta^2(z_n - z) \right)_{\text{PQ}}. \]  
(5)

For a lattice simulation involving the full determinant of the QCD Dirac operator this leads to substantial problems: For \(\mu\) larger than the critical \(\mu\) for pion condensation in phase quenched QCD the eigenvalues \(z_n\) of \(D_\eta \gamma_0 + \mu \gamma_0\) lie arbitrarily close to \(-m\). The complex phase of \((z_n + m)\) therefore is extremely sensitive to the gauge field configuration and this manifests itself in the fluctuation of the phase of the fermion determinant. For this reason the reweighting methods are exceedingly delicate for values of \(\mu\) and \(T\) where phase quenched QCD is in the pion phase. In the light of this, it is unfortunate that the predictions for the critical endpoint in both \(\text{[8]}\) and \(\text{[9]}\) are so close to the predicted phase transition for phase quenched QCD.

**CONCLUSIONS**

In order to emphasize the physical importance of the sign problem for present lattice calculations at non-zero baryon chemical potential we have replotted previously published lattice data in units where a direct comparison to phase quenched QCD is possible. We have observed that the seriousness of the sign problem, as measured by the variance of the phase of the fermion determinant, depends on the distance in the \((2\mu/m_\pi, T/T_0)\)-plane from pion phase transition in phase quenched QCD. The estimate used for the position of the phase transition in phase quenched QCD is independent of any phenomenological parameters. It is obtained as the limit of small quark masses with \(\mu/m_\pi\)-fixed of the result from a random matrix model. While this result is in reasonable agreement with other phenomenological models one should only take it as a rough guideline for the position of the pion phase transition in phase quenched QCD. Lattice simulations of phase quenched QCD can measure the position as well as the order of the phase transition and thus allow for a direct comparison between QCD and phase quenched QCD.

Using the result for the Taylor expansion of the quark number susceptibility in \(\text{[5]}\) we have verified that the number of terms needed in the Taylor expansion approach depends on the seriousness of the sign problem as measured by the variance of the phase of the fermion determinant. The need for a Taylor expansion to \(2n\)th order post a demand for sufficient numerical accuracy to realize cancellations between terms of order \(V^n\) in order to obtain an expectation value of order \(V^0\). Thus the sign problem sets the practical upper bound on the applicability of the Taylor expansion approach. In particular it will be extremely computationally demanding.

\(^1\) I thank Misha Stephanov for suggesting this comparison.
to determine observables in QCD by means of a Taylor expansion if the values of $\mu$ and $T$ are such that phase quenched QCD is in the pion phase.

The need for a high order Taylor expansion to penetrate regions of the $(\mu, T)$-plane where the sign problem is strong also sets a practical limit on the imaginary chemical potential approach. The analytic continuation from imaginary to real chemical potential is carried out by fitting a polynomial in $\mu$ and the order of the polynomial needed corresponds to that of the Taylor expansion. We have checked that no data points have been reported in the literature with this method for values of $\mu$ and $T$ where phase quenched QCD is in the pion condensed phase.

Finally, we have observed that the location of the endpoints of the first order chiral phase transition determined using the reweighting method in $\pi T$ as well as in $\mu T$ falls surprisingly close to the location of the pion phase transition in the phase quenched theory. Despite attempts, no analytical argument to date suggests that this should be the case. For values of $T$ and $\mu$ where the phase quenched theory enters the pion phase the reweighting approach is expected to be extremely delicate. Hence, one may worry that the critical point in $\pi T$ as well as in $\mu T$ are manifestations of the numerical difficulties encountered rather than a true physical effects. Certainly it would be interesting if by an appropriate choice of quark masses one could separate the prediction for the critical point in QCD from the phase boundary in phase quenched QCD. As suggested in [11] fine tuning the quark masses close to critical value for which the chiral transition at $\mu = 0$ becomes first order may cause the endpoint to move to smaller values of $2\mu/m_\pi$.

Acknowledgments: It is a pleasure to thank the participants in and organizers of the KITP program Modern challenges for lattice gauge theory for many stimulating discussions and clarifying answers. In particular Maria Paula Lombardo, Dominique Toublan, Misha Stephanov, Owe Philipsen, Philippe de Forcrand, Jac Verbaarschot and Don Sinclair are thanked. In addition I am grateful to Simon Hands and Shinji Ejiri for challenging discussions and sharing data files.

[1] C.R. Allton, S. Ejiri, S.J. Hands, O. Kaczmarek, F. Karsch, E. Laermann and C. Schmidt, Phys. Rev. D 68 (2003) 014507.
[2] C.R. Allton, S. Ejiri, S.J. Hands, O. Kaczmarek, R.V. Gavai and S. Gupta, Phys. Rev. D 64 (2001) 074506; R.V. Gavai and S. Gupta, Phys. Rev. D 68 (2003) 034506; R.V. Gavai, S. Gupta and R. Roy, Prog. Theor. Phys. Suppl. 153 (2004) 270; R.V. Gavai, S. Gupta and P. Majumdar, Phys. Rev. D 65 (2002) 054506.
[3] R.V. Gavai and S. Gupta, hep-lat/0412035.
[4] C. R. Allton et al., Phys. Rev. D 71 (2005) 054508.
[5] I. M. Barbour, S. E. Morrison, E. G. Klepfish, J. B. Kogut and M. P. Lombardo, Nucl. Phys. Proc. Suppl. 60 A (1998) 220.
[6] Z. Fodor and S. D. Katz, Phys. Lett. B 534 (2002) 87.
[7] Z. Fodor and S. Katz, JHEP 0203 (2002) 014.
[8] Z. Fodor and S. Katz, JHEP 0404 (2004) 050.
[9] A. Hart, M. Laine and O. Philipsen, Phys. Lett. B 505 (2001) 141. P. de Forcrand and O. Philipsen, Nucl. Phys. B 642 (2002) 290;
[10] P. de Forcrand and O. Philipsen, Nucl. Phys. B 673 (2003) 170; O. Philipsen and Ph. de Forcrand, hep-lat/0409034.
[11] M.-P. Lombardo, Nucl. Phys. Proc. Suppl. 83 (2000) 375; M. D’Elia, M.-P. Lombardo, Phys. Rev. D 67 (2003) 014505; M. D’Elia and M.P. Lombardo, Phys. Rev. D 70 (2004) 074509.
[12] K. Splittorff, D. Toublan, J.J.M. Verbaarschot, Nucl. Phys. B 639 (2002) 524.
[13] J.B. Kogut and D.K. Sinclair, Phys. Rev. D 66 (2002) 034505 and Phys. Rev. D 70 (2004) 094501.
[14] B. Klein, D. Toublan and J. J. M. Verbaarschot, Phys. Rev. D 68 (2003) 014009.
[15] L. He, M. Jin, P. Zhuang, hep-ph/0503272.
[16] B. Vanderheyden, A. D. Jackson, Phys. Rev. D 64 (2001) 074016.
[17] Y. Nishida, Phys. Rev. D 69 (2004) 094501.
[18] K. Splittorff, J. T. Lenaghan and J. Wirstam, Phys. Rev. D 67 (2003) 105011.
[19] S. Ejiri, Phys. Rev. D 69 (2004) 094506.
[20] J. C. Osborn, Phys. Rev. Lett. 93 (2004) 222001.
[21] G. Akemann, J. C. Osborn, K. Splittorff and J. J. M. Verbaarschot, Nucl. Phys. B 712 (2005) 287.
[22] J.C. Osborn, K. Splittorff, J.J.M. Verbaarschot, hep-th/0501210, accepted for publication in Phys. Rev. Lett.