3-flavour lattice QCD at finite density and temperature: QCD at finite isospin density revisited*

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Abstract

We simulate 3-flavour lattice QCD at finite temperature and isospin chemical potential $\mu_I$. In particular we study the nature of the finite temperature transition for quark masses close to the critical mass at which this transition for zero chemical potentials changes from a first order transition to a crossover. We find that the Binder cumulants, used to determine the position of this transition, have very strong $dt$ dependence. This leads us to an estimate of the critical mass which is about 20% below previous estimates. In addition, when this $dt$ dependence is taken into account, we find that the Binder cumulants show very little dependence on $\mu_I$. From this we conclude that we do not as yet see any evidence for the expected critical endpoint. We have argued previously that the position and nature of the finite temperature transition for small $\mu_I$ should be the same as that for small quark-number chemical potential $\mu$.

1 Introduction

QCD at finite baryon-number density and temperature was present in the early universe and is produced in relativistic heavy-ion colliders. QCD at finite baryon-number density and zero temperature describes nuclear matter, such as is found in neutron stars.

Because QCD at a finite chemical potential $\mu$ for quark number has a complex determinant, standard simulation methods, based on importance sampling, fail. At small $\mu$, in the neighbourhood of the finite temperature transition, various approaches have been devised to circumvent these problems. These methods include reweighting [1], analytic continuation [2, 3, 4] and series expansions [5, 6]. We adopt a simpler approach and simulate with at a finite isospin chemical potential $\mu_I$ [7]. This corresponds to simulating with finite quark-number chemical potential $\mu = \mu_I/2$ using only the magnitude of the fermion determinant and ignoring its phase. For $\mu$ sufficiently small, this phase is well enough behaved on the sizes of lattice needed for the simulations, that one might expect that the position and nature of the transitions at finite $\mu$ and those at finite $\mu_I$ should be the same.

For 3 flavours of quarks, at zero chemical potentials, there is a critical mass $m_c$ such that the finite temperature transition is first order for $m < m_c$, second order in the 3-d Ising model universality class at $m = m_c$ and becomes a crossover for $m > m_c$ [8] (see also [9, 2]). Here it was expected that, as $|\mu|$ or $|\mu_I|$ was increased, $m_c$ would also increase, providing a critical endpoint at some small chemical potential.

We are performing simulations with $m$ close to $m_c$ on $8^3 \times 4$ and $12^3 \times 4$ lattices. What we find is that the fourth order Binder cumulants, which are used to determine the nature of the transition,

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are very sensitive to the updating increment $dt$ used in the hybrid molecular-dynamics (R algorithm) simulations \[10\]. When this dependence is taken into account, $m_c \lesssim 0.027$ compared with previous estimates of $m_c \approx 0.033$. In addition we have determined that the Binder cumulants have very little $\mu_I$ dependence. Thus, as yet, we have obtained no evidence for a critical endpoint. Both these observations are in agreement with the new results of de Forcrand and Philipsen \[11\].

In section 2 we describe our simulations and present our results. Discussions and conclusions are presented in section 3.

2 Simulations and Results

![Fig. 1: Mass dependence of $B_4(\bar{\psi}\psi)$ for various values of the updating increment $dt$.](image)

The staggered quark action for lattice QCD at finite $\mu_I$ is

$$S_f = \sum_{\text{sites}} \left\{ \bar{\chi} \left[ \frac{1}{2} D(\tau_3 \mu_I) + m \right] \chi + i \lambda \epsilon \bar{\chi} \tau_2 \chi \right\}, \quad (1)$$

which yields a real positive fermion determinant. We simulate this theory with 3 flavours of light dynamical quarks on $8^3 \times 4$ and $12^3 \times 4$ lattices using hybrid molecular-dynamics (R algorithm) methods, in the vicinity of the finite temperature transition. Since we are interested in small $\mu_I$ ($\mu_I < m_{\pi}$) we set $\lambda = 0$.

We run at several quark masses in the range $0.025 \leq m \leq 0.04$, that is, close to the critical mass. The position of the transition is determined by the minimum of the fourth-order Binder cumulant \[12\] for the chiral condensate, defined by

$$B_4(\bar{\psi}\psi) = \frac{\langle (\bar{\psi}\psi - \langle \bar{\psi}\psi \rangle)^4 \rangle}{\langle (\bar{\psi}\psi - \langle \bar{\psi}\psi \rangle)^2 \rangle^2}, \quad (2)$$

where the overline indicates an average over the lattice. 5 noisy estimators of $\bar{\psi}\psi$ are made at the end of each trajectory, which yields an unbiased estimator for $B_4(\bar{\psi}\psi)$. We have checked that this method
for determining the position of the transition produces an estimate which is consistent with the position of the maximum of the corresponding susceptibility. This measurement is obtained by simulating at typically 4 values of $\beta = 6/g^2$ in the neighbourhood of the transition for a given mass, $\mu_I$ (and $dt$), and continuing to the minimum using Ferrenberg-Swendsen reweighting [13]. These simulations are usually 160,000 length-1 trajectories long for each $(m, \beta, \mu_I)$.

Because $B_4$ depends strongly on the updating increment $dt$, we have performed simulations for several different $dt$s in the range $0.01 \leq dt \leq 0.0625$ for each $(m, \mu_I)$. Figure 2 shows the Binder cumulants as functions of mass for the various $dt$ values used, for our $12^3 \times 4$ runs. As we can see, the $dt$ dependence is considerable. At the critical mass, $B_4$ should take the Ising value ($1.604(1)$). If we estimate this from our $dt = 0.05$ simulations we would conclude that $m_c \approx 0.0335$. If on the other hand we use our $dt = 0.02$ runs we predict $m_c \approx 0.027$. Thus we conclude that $m_c \lesssim 0.027$.

Figure 2 shows the $\mu_I$ dependence of $B_4$ for $m = 0.035$ over the range $0 \leq \mu_I \leq 0.3$ ($m_\pi \sim 0.4$), also on a $12^3 \times 4$ lattice. What we see is that, for larger $dt$ values, $B_4$ appears to decrease with increasing $\mu_I$, which would lead us to the erroneous conclusion that there was a critical endpoint where $B_4$ passes through the Ising value for some $\mu_I < 0.2$. As $dt \to 0$, this falloff becomes less pronounced, and there is even the possibility that $B_4$ increases with increasing $\mu_I$. Thus we find no evidence for a critical endpoint.

In figure 3 we plot the values of $B_4$ at $m = 0.035$ and $\mu_I = 0$ against $dt^2$. From this it is clear that, at the smallest $dt$s, $B_4$ is close to its $dt = 0$ value. As we go to larger $dt$, $B_4$ decreases making the transition appear more abrupt, i.e. less like a crossover and more like a first-order transition. Also included in this figure are the chiral susceptibilities, showing their strong $dt$ dependence. These increase with increasing $dt$, again making the transition appear more abrupt.

The transition $\beta$, $\beta_c$ and hence the transition temperature decrease slowly as $\mu_I$ is increased. Our best fit to our measurements of the $\mu_I$ dependence of $\beta_c$ at $m = 0.035$ from our $dt = 0.02$ runs gives

$$\beta_c \approx 5.15193 - 0.1758 \mu_I^2.$$  (3)
This is in reasonable agreement with the estimate at finite $\mu$ of de Forcrand and Philipsen \cite{2,11}, if we make the suggested replacement $\mu_I = 2\mu$.

3 Discussion and Conclusions

We are performing simulations of 3-flavour lattice QCD, using the hybrid molecular-dynamics (R) algorithm, at small isospin chemical potential, close to the finite temperature transition from hadronic/nuclear matter to a quark-gluon plasma. The quark mass is chosen to be close to the critical value for zero chemical potentials. The $\beta$ and hence temperature of this transition decrease slowly with increasing $\mu$, in a manner consistent with the decrease with increasing $\mu_I$, provided one identifies $\mu_I = 2\mu$.

The nature of the transition is determined using Binder cumulants for the chiral condensate. We find that the these cumulants depend strongly on the updating increment $dt$, decreasing with increasing $dt$. This can be understood from the fact that the shift in effective $\beta$ at finite $dt$ is much larger below the transition than above it. Hence a small change in $\beta$, which takes the system through the transition, produces a much larger change in the effective $\beta$. This in turn induces a larger change in observables, which makes the transition appear more abrupt, which is reflected in a smaller value for $B_4$. When this dependence is taken into account, the critical mass is found to be some 20% below previously published values. This is in agreement with the new results obtained by de Forcrand and Philipsen using RHMC (exact) simulations \cite{11}.

When we apply the finite $dt$ corrections to our measurements of the Binder cumulants at finite $\mu_I$, we find that they show little dependence on $\mu_I$. So far, we find no evidence for the predicted critical endpoint. This too is in agreement with the work of de Forcrand and Philipsen, whose new predictions of the nature of the transition at finite $\mu$ obtained from continuations from imaginary $\mu$ also show a weak dependence of $B_4$ on $\mu$ \cite{11}. In fact, their predictions suggest that $B_4$ might actually increase with $\mu$ as was suggested by some of our early results.

We are continuing our simulations at a quark mass of $m = 0.03$ which is closer to the newly
determined critical mass, and at $m = 0.025$ which appears to be just below the critical value. We too are converting to the new RHMC algorithm [14], which is exact. That is, it produces results which do not have any finite $dt$ errors.

If no critical endpoint is found, it will indicate that the critical endpoint, if it exists, is unrelated to that found at zero chemical potentials, as the mass is varied.

We intend to use simulations at finite $\mu_I$ as a platform for reweighting (by the fermion phase factor) to finite $\mu$. This has been found to be a better choice than reweighting from zero $\mu$. Presumably this is because the position of the finite temperature phase transition is the same (or at least close) for the 2 theories. In this respect it has similarities with the method of reweighting from shifted $\beta$ values, used by Fodor and Katz. Here we expect that new methods for simulating fermions will give us at least stochastic estimators for (the phase of) the fermion determinant, removing the burden of exact determinant calculations, which are too expensive.

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