Finite $dt$ dependence of the Binder cumulants for 3-flavor QCD at finite temperature and isospin density

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Abstract

We simulate 3-flavour lattice QCD at small isospin chemical potential $\mu_I$ and finite temperature $T$. At $\mu_I = 0$ there is a critical mass $m_c$ where the finite-temperature transition changes from first order to a crossover. We measure the $\mu_I$ dependence of the transition $\beta (\beta_c)$ for $m$ close to $m_c$, $\beta_c$ and hence $T_c$ decrease slowly with increasing $\mu_I$. $\beta_c$ at finite $\mu_I$ is in good agreement $\beta_c$ at finite $\mu$ (quark-number chemical potential). We use fourth-order Binder cumulants to determine the nature of this transition and to search for a critical endpoint. We measure the $dt$ dependence of these cumulants and extrapolate to $dt = 0$. ($dt$ is the ‘time’ increment used in the hybrid molecular-dynamics simulations.) Preliminary measurements of these Binder cumulants show little $\mu_I$ dependence. (Simulations at imaginary $\mu$ indicate that the $\mu$ dependence of the Binder cumulants is also weak.) This contrasts to the $\mu_I$ dependence we observed at fixed $dt$. 

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I. INTRODUCTION

Although this is nominally the writeup of the talk delivered by JBK at the Workshop on QCD in Extreme Environments, we have taken the liberty of updating our results to reflect the ‘data’ from simulations performed since then. We have done this, since studies of the \( dt \) dependence of observables indicate that the Binder cumulants for the chiral condensate have a strong enough dependence on \( dt \) to change our conclusions. For our earlier results one should see our contribution to Lattice 2004, Fermilab [1].

QCD at finite baryon/quark-number density and temperature is relevant to the physics of relativistic heavy-ion collisions. The various accelerators which probe this region of the phase diagram of nuclear matter include RHIC, CERN heavy-ion, AGS and SIS. Between them they should map out a considerable region of this phase diagram.

QCD and in particular Lattice QCD, at a finite chemical potential \( \mu \) for quark-number, have a complex fermion determinant with a real part of indefinite sign. For this reason standard simulation methods based on importance sampling cannot be applied directly. Various methods have been developed to circumvent this problem for small \( \mu \) in the neighborhood of the finite temperature transition [2, 3, 4, 5, 6, 7, 8, 9, 10]. The transition \( \beta_s \) and hence temperatures for finite \( \mu \) and for finite \( \mu_I \) appear to be the same provided \( \mu_I = 2\mu \). This equality was noted by the Bielefeld-Swansea group [5] and observed by us for the 2-flavor case [11]. Thus the phase of the determinant appears to be unimportant for determining the position of the transition. We have argued that this was because the fluctuations in the phase of the fermion determinant are moderate for small \( \mu \) and high temperatures, on the lattice sizes we use. We speculate that the nature of the transition might also be insensitive to the phase of the determinant. If so, simulations at finite \( \mu_I \) offer an alternative way to study the finite temperature transition at finite \( \mu \). Lattice QCD at finite \( \mu_I \) has a positive fermion determinant, so standard simulation methods work.

We are now extending our simulations to the 3-flavor case. Here we ignore the complication that at finite \( \mu_I \), this theory really describes QCD with \( 3/2 \) \( u \) quark flavors and \( 3/2 \) \( d \) quark flavors. This theory can be interpreted as 3-flavor QCD at finite \( \mu = \mu_I / 2 \) where we use only the magnitude of the fermion determinant and ignore the phase. 3 flavors are of interest because they are closer to the physical \( 2 + 1 \) flavors. In addition, for quark mass \( m < m_c \), the phase transition is first order at \( \mu = \mu_I = 0 \) becoming a crossover for \( m > m_c \)
It is argued that the critical point at $m = m_c$ moves continuously to higher quark mass as $\mu$ is increased, where it becomes the sought-after critical endpoint $[6, 8]$. Choosing a quark mass just above $m_c$, one should be able to keep the critical endpoint as close to $\mu = 0$ as desired. In particular, one should be able to keep the critical $\mu$ in the range where the $\mu$ and $\mu_I$ transitions are related. Thus we might expect a critical endpoint at small $\mu_I$, which we could determine by direct simulations.

Our initial simulations appeared to show evidence for this critical endpoint $[1]$. However, the Binder cumulants, which we use to determine the nature of the transition, depend strongly on $dt$. We are currently performing simulations to study this dependence to allow extrapolation to $dt = 0$. Indications are that the $\mu_I$ dependence of the $dt = 0$ cumulants is rather weak. This observation is consistent with what was predicted from analytic continuation from imaginary $\mu$ by de Forcrand and Philipsen $[8]$. However, our preliminary measurements favor a slow increase with increasing $\mu_I$ while their measurements favor a slow decrease with increasing $\mu$. Considerable more work will be needed to identify the critical endpoint if it exists.

In section 2 we introduce our formulation of lattice QCD at finite $\mu_I$ and discuss its relationship to QCD at finite $\mu$. Section 3 describes our current simulations of 3-flavor lattice QCD at finite $\mu_I$ and gives preliminary results. In section 4 we give our conclusions and discuss what remains to be done.

II. QCD AT FINITE $\mu_I$

The staggered quark action for lattice QCD at finite isospin chemical potential $\mu_I$ is $[11, 15]$

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

where $D \left( \frac{1}{2} \tau_3 \mu_I \right)$ is the normal staggered $D$ for a staggered fermion field $\chi$ with 2 explicit flavor components, and $\tau$ are the isospin Pauli spin matrices acting on this flavor space, with the links in the $+t$ direction multiplied by $\exp(\frac{1}{2} \tau_3 \mu_I)$ and those in the $-t$ direction multiplied by $\exp(-\frac{1}{2} \tau_3 \mu_I)$. Explicit $I_3$ symmetry breaking is provided by the term proportional to $\lambda$. $\lambda \neq 0$ is only needed for $\mu_I \geq m_\pi$ where, in the low temperature phase, $I_3$ is broken spontaneously by a charged pion condensate.
The fermion determinant is
\[
det \left\{ \left[ \mathcal{D}\left( \frac{1}{2}\mu_I \right) + m \right]^\dagger \left[ \mathcal{D}\left( \frac{1}{2}\mu_I \right) + m \right] + \lambda^2 \right\}.
\] (2)

where in this case \( \mathcal{D} \) is only a \( 1 \times 1 \) matrix in isospin space, which means that we only need use a single flavour-component fermion field in our simulations. This determinant is real and positive allowing us to use standard hybrid molecular-dynamics simulations with noisy fermions, to allow us to tune the number of flavors from 8 down to \( N_f \). Here we will choose \( N_f = 3 \), even though this represents \( 3/2 \) isodoublets and probably does not have a sensible continuum limit.

When \( \lambda = 0 \), this determinant is the magnitude of the fermion determinant at finite \( \mu = \frac{1}{2}\mu_I \), so simulating at finite \( \mu_I \) is equivalent to simulating at finite \( \mu \) using only the magnitude of the determinant and neglecting the phase. Hence, the theory we are considering corresponds to the 3-flavor theory at quark number chemical potential \( \mu \), in which the phase of the fermion determinant has been set to zero. We will argue that for small enough \( \mu \), the phase \( \theta \) of the determinant is well enough behaved, that it does not affect the position of the finite temperature transition.

For simplicity let us consider a gluonic observable \( X \). Its expectation value at finite \( \mu \) is given by the ratio
\[
\langle X \rangle_\mu = \frac{\langle e^{i\theta} X \rangle_{\mu_I=2\mu}}{\langle e^{i\theta} \rangle_{\mu_I=2\mu}}
\] (3)

where \( \theta \) is the phase of the fermion determinant. If the denominator
\[
\langle \cos \theta \rangle_{\mu_I=2\mu}
\] (4)
is reasonably large and varies smoothly as \( \beta \) crosses the transition at fixed \( \mu_I \), i.e. it varies considerably more slowly than \( \langle X \rangle \) for the volume considered, it will not have much effect on the transition. We can therefore consider \( e^{i\theta} X \) as our observable and, to the extent to which the position of the transition is independent of the observable, the finite \( \mu \) transition and the finite \( \mu_I \) transition will be coincident. It is not unreasonable to assume that the nature of the two transitions will also be the same. Because this argument only works for finite volumes, it should be considered as a plausibility argument rather than a proof.
III. SIMULATIONS AT SMALL $\mu_I$ AND FINITE TEMPERATURE

We are simulating the 3-flavor theory at finite temperature and small $\mu_I$, i.e. $\mu_I < m_\pi$, since the transition to the phase where isospin ($I_3$) is broken by a charged pion condensate occurs at $\mu_I = m_\pi$ for zero temperature. Since no such condensed phase exists for QCD at finite $\mu$, the physics at finite $\mu$ and that at finite $\mu_I$ can at best be related for $\mu_I < m_\pi$ ($\mu < m_\pi/2$).

Our simulations are being performed on $N_t = 4$ lattices where the zero-chemical-potential finite-temperature phase transition is first order for $m < m_c(0)$ and a crossover for $m > m_c(0)$, with $m_c(0) \approx 0.033$. At $m = m_c(0)$, the transition is a critical point in the universality class of the 3-dimensional Ising model. As $\mu$ is increased, $m_c$ is expected to increase so that the $m_c(\mu)$ becomes the critical endpoint. Fixing $m$ to lie just above $m_c(0)$, the transition should be a crossover for $\mu < \mu_c$ with $\mu_c(m)$ the solution of $m = m_c(\mu_c)$. For $\mu > \mu_c$, the transition should become first order. The critical endpoint should again lie in the Ising universality class. From the observation that the $\mu$ and $\mu_I$ transitions seem to be related, one might expect a corresponding endpoint for finite $\mu_I$.

We are performing simulations at $m = 0.03$, $m = 0.035$ and $m = 0.04$. Most of our effort has been concentrated on $m = 0.035$, just above $m_c(0)$, where we might hope to find a critical endpoint for small $\mu_I$. Our simulations are being performed on $8^3 \times 4$, $12^3 \times 4$ and $16^3 \times 4$ lattices.

Figure 1 shows the Wilson line from our $8^3 \times 4$ simulations at $m = 0.035$ for several values of $\mu_I < m_\pi$. The values of $dt$ used for each of the $\mu_I$ values used in these simulations are $dt = 0.05$ for $\mu_I = 0.0, 0.2$, $dt = 0.04$ at $\mu = 0.25$, $dt = 0.03125$ for $\mu_I = 0.03$ and $dt = 0.02$ at $\mu_I = 0.0375$. The length of the simulations for each of those $\beta$ values closest to the transition for each $\mu_I$ is 160,000 time-units (trajectories).

We study the nature of these transitions using 4-th order Binder cumulants \[16\]. If $X$ is an observable, its Binder cumulant is defined by

$$B_4(X) = \frac{\langle (X - \langle X \rangle)^4 \rangle}{\langle (X - \langle X \rangle)^2 \rangle^2} \quad (5)$$

The Binder cumulant of interest is that for the chiral condensate. Since we only measure stochastic estimators of the chiral condensate, we need at least 4 independent stochastic estimates of $\langle \bar{\psi} \psi \rangle$ for each configuration to obtain an unbiased estimate of $B_4$ – we actually use 5 noise vectors for each configuration.
FIG. 1: Wilson Lines as functions of $\beta$ for several values of $\mu_I$ on an $8^3 \times 4$ lattice with $m = 0.035$.

On a lattice of infinite spatial extent, $B_4(\langle \bar{\psi} \psi \rangle)$ would be 3 for a crossover and 1 for a first order transition, while for a critical point in the Ising universality class it would have the value 1.604(1). For finite lattices $B_4(\langle \bar{\psi} \psi \rangle)$ will lie above the Ising value in the crossover region and below this value in the first-order regime, passing smoothly through a value close to the Ising value at the critical endpoint. As the size of the spatial lattice is increased, the curve will pass more steeply through the Ising value. The critical endpoint can be obtained by observing where the curves for different lattice sizes cross, or where the curve for a given large lattice passes through the Ising value. Ideally one should use several spatial volumes,
observe where the curves cross, and check that the value of $B_4$ at this point is (close to) the Ising value.

Preliminary indications based on simulations with the $dt$ values given above showed some evidence for such a critical endpoint. However, it was observed that, while the value of $B_4$ fell with increasing $\mu_I < < m_\pi$, it began to increase again long before $m_\pi$. This suggested that we should study the $dt$ dependence of $B_4$. We are now performing a detailed finite $dt$ analysis. What we find is that the $dt$ dependence of the fluctuation quantities – $B_4(\langle \bar{\psi}\psi \rangle)$ and the susceptibility $\chi(\langle \bar{\psi}\psi \rangle)$ – is considerable, something we had also observed in the 2 flavor case at $\mu_I > m_\pi$. The preliminary results of this analysis which we present below indicate that considerable work will be needed to determine whether there is evidence for a critical endpoint, and if so, determine its position.

Figure 2 shows the $dt$ dependence of $B_4$ for the chiral condensate for $m = 0.035$ and $\mu_I = 0$ from our $12^3 \times 4$ runs at $dt$ values of 0.0625, 0.05, 0.04 and 0.03125. Each point is the value of $B_4$ obtained from performing a Ferrenberg-Swendsen extrapolation [17] to its minimum from $\beta$ values close to the transition. We have noted that the values of $\beta_c$ obtained from the minima of $B_4$ and from the maxima of the chiral susceptibility are consistent. We have averaged the results obtained from 2 or 3 different $\beta$ values close to the transition, for each $dt$. The length of the runs at each $\beta$ was 160,000 $\Delta t = 1$ trajectories. We also noted that the values of $\beta_c$ obtained from different $\beta$s and the same $dt$ were consistent. We note considerable variation of $B_4$ over the range of $dt$s used in these runs. A fit linear in $dt^2$ gives $B_4(dt = 0) = 1.84(3)$ with a $\chi^2/dof$ of 0.6. This shows that, for $dt = 0.0625$ the finite $dt$ error $\approx 16.5\%$. Even at $dt = 0.05$ which we used for our earlier simulations the error $\approx 9\%$. This also shows that finite $dt$ errors can take one from $B_4 > 1.604$, which is normally interpreted as a crossover to $B_4 < 1.604$ which is commonly interpreted as indicative of a first order transition.

We are performing similar calculations of the finite $dt$ dependence of $B_4$ for the chiral condensate for $\mu_I > 0$. Preliminary results are shown in figure 3. Again we see a strong dependence of $B_4$ on $dt$. Because $\mu_I \neq 0$ makes the Dirac operator more singular, smaller $dt$ values are required as $\mu_I$ is increased. An extrapolation linear in $dt^2$ to $dt = 0$ gives $B_4 = 1.89(3)$ for $\mu_I = 0.2$ and $B_4 = 2.01(8)$ for $\mu_I = 0.3$. The rise in $B_4$ with increasing $\mu_I$, although suggestive, is not statistically significant. All we can claim at present is that there is little if any dependence of $B_4(\langle \bar{\psi}\psi \rangle)$ on $\mu_I$ over this range. For completeness we plot these
FIG. 2: Estimates of $B_4(\langle \bar{\psi} \psi \rangle)$ as a function of $dt^2$ at $m = 0.035$ and $\mu_I = 0$ on a $12^3 \times 4$ lattice.

The values of $\beta_c$, the transition $\beta$ are calculated from the minima of $B_4$. We have noted that these estimate of $\beta_c$ are in excellent agreement with those obtained from the maxima of the susceptibilities for the chiral condensate. Extrapolating these to $dt = 0$, linearly in $dt^2$, we obtain the results shown in figure 5. The statistical errors are small, but there are large systematics associated with this preliminary ‘data’. The straight line fit shown in the figure is:

$$\beta_c = 5.15195 - 0.19428 \mu_I^2.$$  \hspace{1cm} (6)

We do not quote any errors because of the preliminary nature of this result. If we interpret $\mu_I = 2\mu$ as we have suggested, this is in good agreement with the measurements of de
FIG. 3: Estimates of \( B_4(\langle \bar{\psi} \psi \rangle) \) as a function of \( dt^2 \) at \( m = 0.035 \) on a \( 12^3 \times 4 \) lattice a) for \( \mu_I = 0.2 \) and b) for \( \mu_I = 0.3 \).

Forcrand and Philipsen [8].

It is helpful to consider why the transition appears more like a first-order transition as \( dt \)
FIG. 4: Estimates of $B_4(\langle \bar{\psi}\psi \rangle)$ extrapolated to $dt = 0$, as functions of $\mu_I$ on a $12^3 \times 4$ lattice.

is increased from zero. A brief discussion of this was given in our 2-flavor paper \[11\]. One of the effects of simulating at a finite $dt$ using the hybrid molecular-dynamics method, which is an inexact algorithm, is that the effective $\beta$ value $\beta_{\text{effective}}$ measured from the kinetic term in the molecular-dynamics Hamiltonian using the equipartition theorem is (on the average) less than the input $\beta$, so that we are effectively running at a lower $\beta$ value. The quantity $\Delta \beta = \beta - \beta_{\text{effective}}$ increases with increasing $dt$. This would not be a problem if the shift were roughly constant as $\beta$ was varied across the transition. However, this is not the case for a constant $dt$. $\Delta \beta$ is significantly larger below the transition than above. We illustrate this from our simulations at $\mu_I = 0$, $m = 0.035$, $\lambda = 0$ and $dt = 0.05$ on an $8^3 \times 4$ lattice,
where we have ‘data’ at a number of $\beta$ values over a range which includes the transition. This is shown in figure 6.

Now let us consider what the effect of such $\beta$ dependence for $\Delta \beta$ has on the behavior of the simulation close to the transition. Here, a small change in $\beta$ causes a relatively large change in $\beta_{\text{effective}}$. This causes a relatively large change in all observables. This, in turn, makes the transition appear more abrupt and hence nearer to being first-order. Looking at this in another way, $\beta_{\text{effective}}$ needs to undergo a relatively large fluctuation to take it from one side of the transition to the other. This makes it more difficult for the system to fluctuate between its low-$\beta$ domain and its high-$\beta$ domain. Such a tendency to
FIG. 6: $\Delta \beta = \beta - \beta_{\text{effective}}$ as a function of $\beta$ at $\mu_I = 0$, $m = 0.035$, $\lambda = 0$ and $dt = 0.05$ on an $8^3 \times 4$ lattice.

remain in one domain or the other, only ‘tunneling’ between domains rather infrequently, is a property one associates with first-order behavior. Hence the transition will appear to be closer to a first-order transition than it really is. These considerations are in accord with our observations.
IV. DISCUSSION AND CONCLUSIONS

We are simulating 3-flavor lattice QCD with a chemical potential $\mu_I$ for isospin ($I_3$), at small $\mu_I$ and temperatures close to the finite temperature transition from hadronic/nuclear matter to a quark-gluon plasma. These simulations are being performed on $8^3 \times 4$, $12^3 \times 4$, and $16^3 \times 4$ lattices. In this regime, the behavior of QCD at finite $\mu_I$ and that at finite quark-number chemical potential $\mu$ appear similar for $\mu_I = 2\mu$. QCD at finite $\mu$ and QCD at finite $\mu_I$ are related if one can neglect the phase angle of the determinant, or include it in the observables. The decrease in $\beta_c$ with increasing $\mu_I$ that we have observed is consistent with that seen by de Forcrand and Philipsen if we make the substitution $\mu = \frac{1}{2} \mu_I$, which adds further support to the proposition that finite $\mu$ and finite $\mu_I$ are related.

At zero chemical potentials there exists a critical mass $m_c$. For $m < m_c$ the finite temperature transition is first order. For $m > m_c$ this transition is a mere crossover, with no real phase transition. At $m = m_c$ the transition is a critical point in the universality class of the 3-dimensional Ising model. For staggered lattices with $N_t = 4$, $m_c \approx 0.033$. It has been suggested that at finite $\mu$, the critical mass $m_c(\mu)$ moves continuously (in $\mu$) to higher values, where it becomes the critical endpoint. Hence the best place to look for a critical endpoint in $\mu$ or $\mu_I$ should be for a quark mass just above $m_c$ where it would be expected to be found at a small chemical potential. For this reason most of our simulations have been performed at $m = 0.035$.

We have used 4-th order Binder cumulants for the chiral condensate to determine the nature of the finite temperature transition. A critical endpoint would be where the Binder cumulants for different lattice sizes cross. At this point its value should be close to the Ising value 1.604(1). Although our preliminary results appeared to show evidence for such an endpoint, further simulations studying the finite $dt$ dependence of this cumulant showed the finite $dt$ errors to be large at the $dt$s we were using. Our current estimates show the extrapolated cumulants to lie well above the Ising value for the $\mu_I$ range being considered. There is no indication that these cumulants are falling with increasing $\mu_I$. In fact our measurements show a slight rise with increasing $\mu_I$. However, this rise is not statistically significant, especially considering that these preliminary measurements could have sizable systematic errors. All that we can claim is that the $\mu_I$ dependence of the Binder cumulants is very weak over this range. This is in qualitative agreement with what was observed at
finite $\mu$ by de Forcrand and Philipsen, who observed a slight decrease in $B_4$ with increasing $\mu^2$, but could not exclude a $B_4$ which is independent of $\mu^2$.

If we do not find evidence for a $B_4$ which decreases with increasing $\mu_I$ at this quark mass, we should check the situation even closer to $m_c$. The lack of any critical end point, even for $m$ much closer to (but still above) $m_c$ would suggest that similar behavior would be found at small $\mu$, since our estimates of the fluctuations of the phase angle as determined from $\langle \cos \theta \rangle$ ($\theta$ is the phase of the fermion determinant at $\mu = \frac{1}{2} \mu_I$) indicate that it is reasonably well behaved for $m = 0.035$ over most of the region $\mu_I < m_{\pi}$ for an $8^3 \times 4$ lattice. This, in turn, would suggest that the critical endpoint at finite $\mu$ (if it exists) is fluctuation induced. Thus we would expect to find it where fluctuations in $\theta$ become large, i.e. for $\mu \gtrsim m_{\pi}/2$. If so, it would not move continuously away from $\mu = 0$ as $m$ becomes larger than $m_c$, but might be expected to jump from $\mu = 0$ to $\mu \approx m_{\pi}/2$, as $m$ is increased beyond $m_c$.

The strong dependence of $B_4$ on $dt$ suggests that we should investigate the use of recently formulated exact algorithms (see [18] and references contained therein), for our simulations. Since such methods rely on stochastic approximations to the fermion determinant, they could also help us in applying reweighting by the phase of the fermion determinant as a way of studying finite $\mu$ in a quantitative fashion, to obtain the equation-of-state. Here we note recent work indicating that finite $\mu_I$ simulations provide a better platform for reweighting than reweighting from simulations at $\mu = 0$ [19].

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