Lattice QCD at finite $T$ and $\mu$ and the critical point of QCD

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We propose a method to study lattice QCD at finite $T$ and $\mu$. We compare it with direct results and with the Glasgow method by using $n_f=4$ QCD at $\text{Im}(\mu)\neq 0$. We locate the critical endpoint (E) of QCD on the Re($\mu$)-$T$ plane. In this study we use $n_f=2+1$ dynamical staggered quarks with semi-realistic masses on $L_t=4$ lattices.

I. Introduction. — QCD at finite $T$ and $\mu$ is of fundamental importance, since it describes relevant features of particle physics in the early universe, in neutron stars and in heavy ion collisions. Extensive experimental work has been done with heavy ion collisions at CERN and Brookhaven to explore the $\mu$-$T$ phase diagram. It is a long-standing non-perturbative question, whether a critical point exists on the $\mu$-$T$ plane, and particularly how to tell its location theoretically [1].

A recent review on QCD at finite $T$ is Ref. [4]. We propose a method to reduce the overlap problem and determine the phase diagram in the $\mu$-T plane “for details see [2].” We also locate the critical point of QCD. (Similar technique was successful for determining the endpoint of the hot electroweak plasma [2] e.g. on 4D lattices.)

II. Overlap improving multi-parameter reweighting. — Let us study a generic system of fermions $\psi$ and bosons $\phi$, where the fermion Lagrange density is $\bar{\psi}M(\phi)\psi$. Integrating over the Grassmann fields we get:

$$Z(\alpha) = \int D\phi \exp[-S_{\text{bos}}(\alpha, \phi)] \det M(\phi, \alpha),$$

where $\alpha$ denotes a set of parameters of the Lagrangian. In the case staggered QCD $\alpha$ consists of $\beta$, the quark mass ($m_q$) and $\mu$. For some choice of the parameters $\alpha=\alpha_0$ importance sampling can be done (e.g. for Re($\mu)=0$). Rewriting the above equation one obtains

$$Z(\alpha) = \int D\phi \exp[-S_{\text{bos}}(\alpha_0, \phi)] \det M(\phi, \alpha_0)$$

$$\left\{ \frac{\text{det} M(\phi, \alpha)}{\text{det} M(\phi, \alpha_0)} \right\}.$$ 

We treat the curly bracket as an observable — which is measured on each configuration — and the rest as the measure. It is known that changing only one parameter of the ensemble generated at $\alpha_0$ provides an accurate value for some observables only for high statistics. This is ensured by rare fluctuations as the mismatched measure occasionally sampled the regions where the integrand is large. This is the so-called overlap problem. Having several parameters the set $\alpha_0$ can be adjusted to ensure a better overlap than obtained by varying only one parameter.

The basic idea of the method as applied to dynamical QCD can be summarized as follows. We study the system at Re($\mu)=0$ around its transition point. Using a Glasgow-type technique we calculate the determinants for each configuration for a set of $\mu$, which, similarly to the Ferrenberg-Swendsen method [5], can be used for reweighting. The average plaquette values can be used
to perform an additional reweighting in $\beta$. Since transition configurations were reweighted to transition configurations a much better overlap can be observed than by reweighting pure hadronic configurations to transition ones as done by the Glasgow-type techniques (moving along the transition line was also suggested by Ref. [10]).

III. Illustration and direct test.— We have directly tested these ideas in four-flavor QCD with $m_q=0.05$ dynamical staggered quarks.

We first collected 1200 independent $V=4 \cdot 6^3$ configurations at $\text{Re}(\mu)=\text{Im}(\mu)=0$ and some $\beta$ values and used the Glasgow-reweighting and also our technique to study $\text{Re}(\mu)=0$, $\text{Im}(\mu)\neq 0$. At $\text{Re}(\mu)=0$, $\text{Im}(\mu)\neq 0$ direct simulations are possible. After performing these direct simulations as well, a clear comparison can be done. Figure 1 shows the predictions of the three methods for the average quark condensates at $\beta=5.085$ as a function of $\text{Im}(\mu)$. The predictions of our method agree with the direct results, whereas for larger $\text{Im}(\mu)$ the predictions of the Glasgow method are by several standard deviations off. Based on these experiences we expect that our method can be successfully applied at $\text{Re}(\mu)\neq 0$.

IV. $n_f \neq 4$ staggered quarks. — In QCD with $n_f$ staggered quarks one should change the determinants to their $n_f/4$ power in our two equations.

Importance sampling works also in this case at some $\beta$ and at $\text{Re}(\mu)=0$. Since $\det M$ is complex, one should choose among the Riemann-sheets of the fractional power. We solved this problem analytically [5].

In the following we keep $\mu$ real and look for the zeros of $Z$ on the complex $\beta$ plane. At a first order phase transition the free energy $\propto \log Z(\beta)$ is non-analytic. Clearly, a phase transition appears only in the $V\to \infty$ limit, but not in a finite $V$. Nevertheless, $Z$ has zeros at finite $V$, generating the non-analyticity of the free energy, the Lee-Yang zeros [8]. These are at complex values of the parameters, in our case at complex $\beta$. For a system with a first order transition these zeros approach the real axis in the $V\to \infty$ limit (detailed analysis suggests $1/V$ scaling). This $V\to \infty$ limit generates the non-analyticity of the free energy. For a system with crossover $Z$ is analytic, and the zeros do not approach the real axis in the $V\to \infty$ limit.

At $T\neq 0$ we used $L_t=4$, $L_s=4,6,8$ lattices. $T=0$ runs were done on $10^3 \cdot 16$ lattices. $m_u,d=0.025$ and $m_s=0.2$ were our bare quark masses.

At $T \neq 0$ we determined the complex valued Lee-Yang zeros, $\beta_0$, for different $V$-s as a function of $\mu$. Their $V\to \infty$ limit was given by $\beta_0(V) = \beta_0^\infty + \zeta/V$ extrapolation. We used 14000, 3600 and 840 configurations on $L_s=4,6$ and 8 lattices, respectively. Figure 2 shows $\text{Im}(\beta_0^\infty)$ as a function of $\mu$. For small $\mu$-s the extrapolated $\text{Im}(\beta_0^\infty)$ is

Figure 1. The average of $\bar{\psi}\psi$ at $\beta=5.085$ as a function of $\text{Im}(\mu)$, for direct results (squares; their sizes give the errors), our technique (crosses) and Glasgow-type reweighting (dots).

Figure 2. $\text{Im}(\beta_0^\infty)$ as a function of the chemical potential.
Figure 3. The T-µ diagram. Direct results are given with errorbars. Dotted line shows the crossover, solid line the first order transition. The box gives the uncertainties of the endpoint.

inconsistent with a vanishing value, and predicts a crossover. Increasing µ the value of \( \text{Im}(\beta_\infty^0) \) decreases, thus the transition becomes consistent with a first order phase transition. (Note, that systematic overshooting is a finite V effect.) The statistical error was determined by jackknife samples of the total \( L_s = 4, 6 \) and 8 ensembles. Our primary result is \( \mu_{\text{end}} = 0.375(20) \).

To set the physical scale we used a weighted average of \( R_0, m_\rho \) and \( \sqrt{\sigma} \). Note, that (including systematics due to finite V) we have \( (R_0 \cdot m_\rho) = 0.73(6) \), which is at least twice, \( m_{u,d} \) is at least four times as large as the physical values.

Figure 3 shows the phase diagram in physical units, thus \( T \) as a function of \( \mu_B \), the baryonic chemical potential (which is three times larger then the quark chemical potential). The endpoint is at \( T_E = 160 \pm 3.5 \) MeV, \( \mu_E = 725 \pm 35 \) MeV. At \( \mu_B = 0 \) we obtained \( T_c = 172 \pm 3 \) MeV.

IV. Conclusions.— We proposed a method – an overlap improving multi-parameter reweighting technique– to numerically study non-zero \( \mu \) and determine the phase diagram in the \( T-\mu \) plane. Our method is applicable to any number of Wilson or staggered quarks. As a direct test we showed that for \( \text{Im}(\mu) \neq 0 \) the predictions of our method are in complete agreement with the direct simulations, whereas the Glasgow method suffers from the well-known overlap problem.

We studied the \( \mu-T \) phase diagram of QCD with dynamical \( n_f=2+1 \) quarks. Using our method we obtained \( T_E = 160 \pm 3.5 \) MeV and \( \mu_E = 725 \pm 35 \) MeV for the endpoint. Though \( \mu_E \) is too large to be studied at RHIC/LHC, the endpoint would probably move closer to the \( \mu = 0 \) axis when the quark masses get reduced. At \( \mu = 0 \) we obtained \( T_c = 172 \pm 3 \) MeV. Clearly, more work is needed to get the final values. One has to extrapolate to zero step-size in the R-algorithm and to the thermodynamic, chiral and continuum limits.

This work was partially supported by Hung. Sci. grants No. OTKA-T34980/T29803/-T22929/M28413/OM-MU-708/IKTA111/NIIF. This work was in part based on the MILC collaboration’s public lattice gauge theory code: http://physics.indiana.edu/~sg/milc.html.

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