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Lattice QCD results at finite T and μ

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Abstract. We propose a method to study lattice QCD at finite temperature (T) and chemical potential (μ). We test the method and compare it with the Glasgow method using n_f=4 staggered QCD with imaginary μ. The critical endpoint (E) of QCD on the Re(μ)-T plane is located. We use n_f=2+1 dynamical staggered quarks with semi-realistic masses on L_t=4 lattices. Our results are based on $\mathcal{O}(10^3 - 10^4)$ configurations.

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1. Introduction

QCD at finite T and/or μ 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 μ-T phase boundary (cf. [1]). Note, that past, present and future heavy ion experiments with always higher and higher energies produce states closer and closer to the T axis of the μ-T diagram. It is a long-standing question, whether a critical point exists on the μ-T plane, and particularly how to tell its location theoretically [2].

Let us discuss the μ=0 case first. Universal arguments [3] and lattice simulations [4] indicate that in a hypothetical QCD with a strange (s) quark mass (m_s) as small as the up (u) and down (d) quark masses ($m_{u,d}$) there would be a first order finite T phase transition. The other extreme case (n_f=2) with light u/d quarks but with an infinitely large m_s there would be no phase transition, only a crossover. Observables change rapidly during a crossover, but no singularities appear. Between the two

extremes there is a critical strange mass (m_s^c) at which one has a second order finite T phase transition. Staggered lattice results on L_t=4 lattices with two light quarks and m_s around the transition T (n_f=2+1) indicated [5] that m_s^c is about half of the physical m_s. Thus, in the real world we probably have a crossover.

Returning to a non-vanishing μ, one realizes that arguments based on a variety of models (see e.g. [6, 7, 2]) predict a first order finite T phase transition at large μ. Combining the $\mu = 0$ and large μ informations an interesting picture emerges on the μ-T plane. For the physical m_s the first order phase transitions at large μ should be connected with the crossover on the $\mu = 0$ axis. This suggests that the phase diagram features a critical endpoint E (with chemical potential μ_E and temperature T_E), at which the line of first order phase transitions ($\mu > \mu_E$ and $T < T_E$) ends [2]. At this point the phase transition is of second order and long wavelength fluctuations appear, which results in (see e.g. [8]) consequences, similar to critical opalescence. Passing close enough to (μ_E,T_E) one expects simultaneous appearance of signatures which exhibit nonmonotonic dependence on the control parameters [9], since one can miss the critical point on either sides.

The location of E is an unambiguous, non-perturbative prediction of QCD. No *ab initio*, lattice analysis based on QCD was done to locate the endpoint. Crude models with $m_s = \infty$ were used (e.g. [2]) suggesting that $\mu_E \approx 700$ MeV, which should be smaller for finite m_s. The goal of our exploratory work is to propose a new method to study lattice QCD at finite μ and apply it to locate the endpoint. We use full QCD with dynamical n_f=2+1 staggered quarks.

QCD at finite μ can be given on the lattice [10]; however, standard Monte-Carlo techniques fail. At Re(μ)$\neq$0 the determinant of the Euclidean Dirac operator is complex, which spoils any importance sampling method.

Several suggestions were studied in detail to solve the problem. We list a few of them (for a recent review see Ref. [11]).

In the large gauge coupling limit a monomer-dimer algorithm was used [12]. For small gauge coupling an attractive approach is the "Glasgow method" [13] in which the partition function is expanded in powers of $\exp(\mu/T)$ by using an ensemble of configurations weighted by the μ=0 action. After collecting more than 20 million configurations only unphysical results were obtained: a premature onset transition. The reason is that the μ=0 ensemble does not overlap sufficiently with the states of interest. Another possibility is to separate the absolute value and the phase of the fermionic determinant and use the former to generate configurations and the latter in observables [14]. The curvature of the $\mu - T$ phase diagram at $\mu = 0$ was determined by a stochastic calculation of the derivatives of the fermion determinant in [15].

At imaginary μ the measure remains positive and standard Monte Carlo techniques apply. The canonical partition function can be obtained by a Fourier transform [16,17]. In this technique the dominant source of errors is the Fourier transform rather than the poor overlap. One can also use the fact that the partition function away from the transition line should be an analytic function of μ, and the fit for imaginary μ values could be analytically continued to real values of μ [18]. At T

sufficiently above the transition, both real and imaginary μ can be studied by dimensionally reducing QCD [19]. Hamiltonian formulation may also help studying the problem [20].

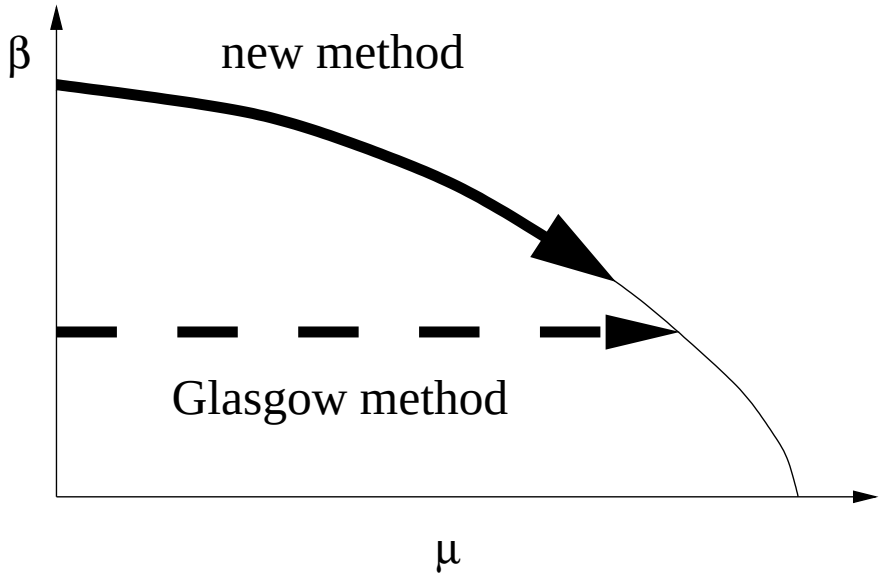

Fig. 1. Schematic difference between the present and the Glasgow methods.

An attractive approach to alleviate the problem is the "Glasgow method" (see e.g. Ref. [13]) in which the partition function (Z) is expanded in powers of $\exp(\mu/T)$ by using an ensemble of configurations weighted by the μ=0 action. After collecting more than 20 million configurations only unphysical results were obtained. The reason is that the μ=0 ensemble does not overlap enough with the finite density states of interest [21].

We propose a method to reduce the overlap problem and determine the phase diagram in the μ-T plane (for details see [22]). The idea is to produce an ensemble of QCD configurations at μ=0 and at the transition temperature T_c. Then we determine the Boltzmann weights [24] of these configurations at $\mu \neq 0$ and at T lowered to the transition temperatures at this non-vanishing μ. Since transition configurations are reweighted to transition ones a much better overlap can be observed than by reweighting pure hadronic configurations to transition ones [13]. Since the original ensemble is collected at μ=0 we do not expect to be able to decsribe the physics of the large μ region with e.g. exotic colour superconductivity. Fortunately, the typical μ values at present heavy ion accelerators are smaller than the region

we cover (for the freeze-out condition see e.g. [25]).

After illustrating the applicability of the method we locate the critical point of QCD. (Multi-dimensional reweighting was successful for determining the endpoint of the hot electroweak plasma [23] e.g. on 4D lattices.)

2. Overlap improving multi-parameter reweighting

Let us study a generic system of fermions ψ and bosons ϕ, where the fermion Lagrange density is $\bar{\psi}M(\phi)\psi$. Integrating over the Grassmann fields we get:

$$Z(\alpha) = \int \mathcal{D}\phi \exp[-S_{bos}(\alpha,\phi)] \det M(\phi,\alpha), \tag{1}$$

where α denotes a set of parameters of the Lagrangian. In the case of staggered QCD α consists of β, m_q and μ. For some choice of the parameters $\alpha{=}\alpha_0$ importance sampling can be done (e.g. for $\mathrm{Re}(\mu){=}0$). Rewriting eq. (1)

$$Z(\alpha) = \int \mathcal{D}\phi \exp[-S_{bos}(\alpha_0,\phi)] \det M(\phi,\alpha_0)$$
$$\left\{ \exp[-S_{bos}(\alpha,\phi) + S_{bos}(\alpha_0,\phi)] \frac{\det M(\phi,\alpha)}{\det M(\phi,\alpha_0)} \right\}. \tag{2}$$

We treat the curly bracket as an observable (measured on each configuration) and the rest as the measure. Changing only one parameter of the ensemble generated at α_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 overlap problem. Having several parameters the set α_0 can be adjusted to get 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 $\mathrm{Re}(\mu){=}0$ around its transition point. Using a Glasgow-type technique we calculate the determinants for each configuration for a set of μ, which, similarly to the Ferrenberg-Swendsen method [24], can be used for reweighting. The average plaquette values can be used to perform an additional reweighting in β. Since transition configurations were reweighted to transition ones a much better overlap can be observed than by reweighting pure hadronic configurations to transition ones as done by the Glasgow-type techniques. The differences between the two methods are shown in Figure 1. Moving along the transition line was also suggested by Ref. [17].

We have directly tested these ideas in $n_f{=}4$ QCD with $m_q{=}0.05$ dynamical staggered quarks. We first collected 1200 independent $\mathrm{V}{=}4{\cdot}6^3$ configurations at $\mathrm{Re}(\mu){=}\mathrm{Im}(\mu){=}0$ and some β values and used the Glasgow-reweighting and also our technique to study $\mathrm{Re}(\mu){=}0$, $\mathrm{Im}(\mu){\neq}0$. At $\mathrm{Re}(\mu){=}0$, $\mathrm{Im}(\mu){\neq}0$ direct simulations are possible. After performing these direct simulations as well, a clear comparison can be done. Figure 2 shows the predictions of the three methods for the average

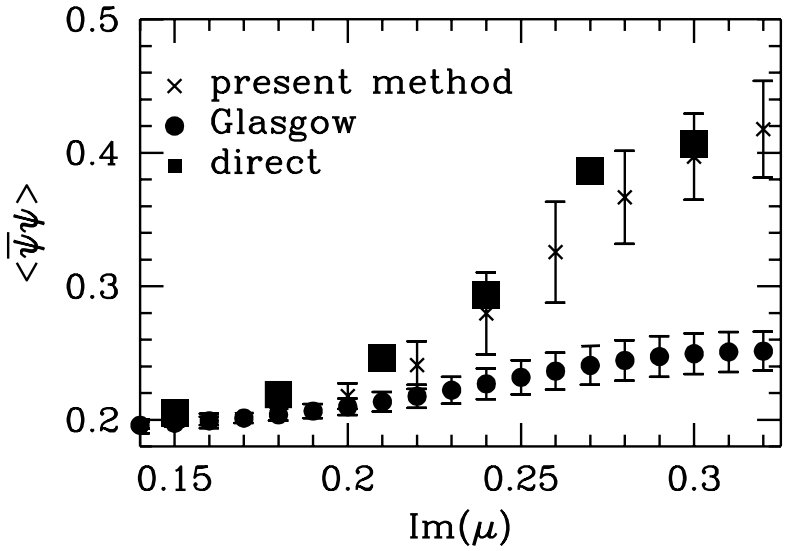

Fig. 2. $\bar{\psi}\psi$ as a function of Im(μ), for direct results (squares), our technique (crosses) and Glasgow-type reweighting (dots).

quark condensates at β=5.085 as a function of Im(μ). The predictions of our method agree with the direct results, whereas for larger Im(μ) the predictions of the Glasgow method are by several standard deviations off. We expect that our method can be applied at Re(μ)$\neq$0.

3. The endpoint of $n_f = 2 + 1$ QCD

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 β and at Re(μ)=0. Since det M is complex an additional problem arises, one should choose among the possible Riemann-sheets of the fractional power in eq. (2). This can be done by using [22] the fact that at μ=μ_w the ratio of the determinants is 1 and it should be a continuous function of μ.

In the following we keep μ real and look for the zeros of Z for complex β. At a first order phase transition the free energy $\propto \log Z(\beta)$ is non-analytic. 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 [26]. These are at complex parameters (e.g. β). For a system with first order

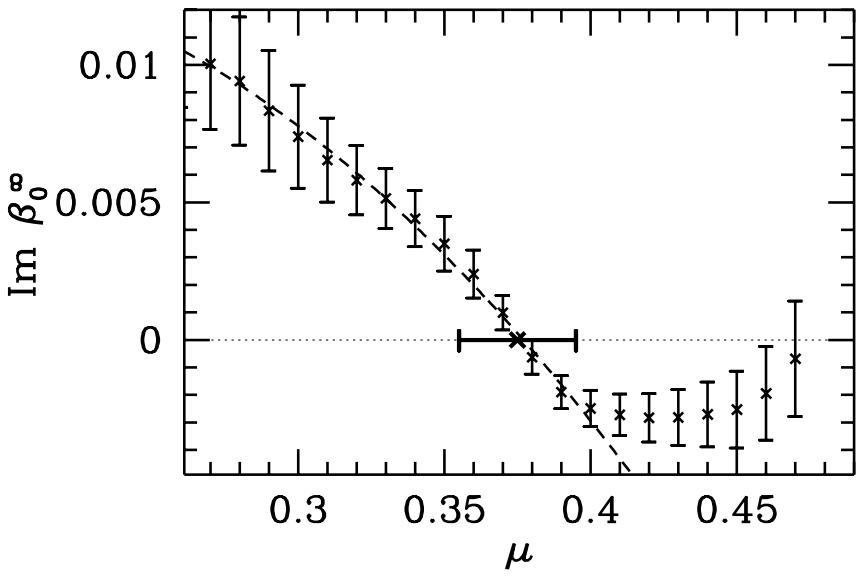

Fig. 3. $\mathrm{Im}(\beta_0^\infty)$ as a function of the chemical potential.

transition these zeros approach the real axis as V$\to\infty$ by a $1/V$ 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 as V$\to\infty$.

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, β_0, for different V-s as a function of μ. Their V$\to\infty$ limit was given by a $\beta_0(V)=\beta_0^\infty+\zeta/V$ extrapolation. We used 14000, 3600 and 840 configurations on L_s=4,6 and 8 lattices, respectively. $\mathrm{Im}(\beta_0^\infty)$ is shown on Figure 3 as a function of μ. For small μ-s the extrapolated $\mathrm{Im}(\beta_0^\infty)$ is inconsistent with a vanishing value, and predicts a crossover. Increasing μ the value of $\mathrm{Im}(\beta_0^\infty)$ decreases, thus the transition becomes consistent with a first order phase transition (overshooting is a finite V effect). Our primary result is $\mu_{end}=0.375(20)$.

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

Figure 4 shows the phase diagram in physical units, thus T as a function of μ_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 μ_B=0 we obtained $T_c=172\pm 3$ MeV.

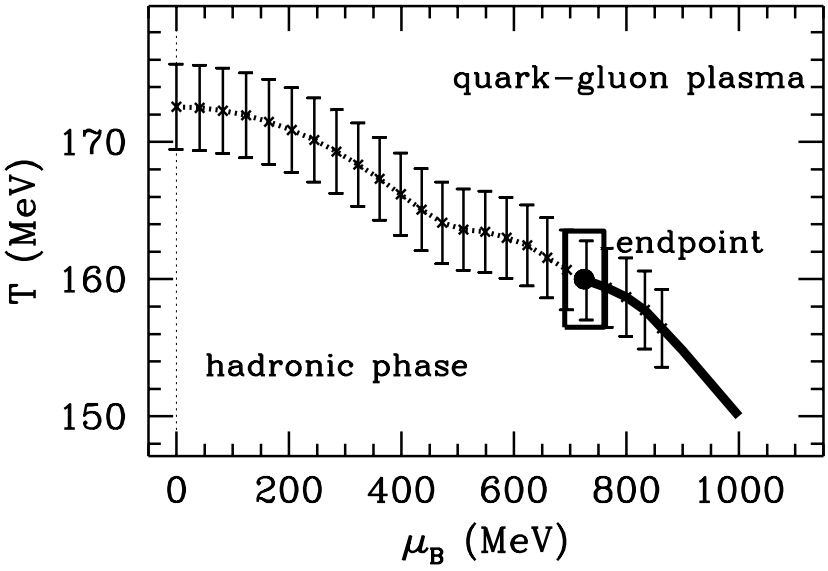

Fig. 4. The T-μ diagram. Direct results are given with errorbars. Dotted line shows the crossover, solid line the first order transition. The box gives the uncertainties of the endpoint.

4. Conclusion

We proposed a method –an overlap improving multi-parameter reweighting technique– to numerically study non-zero μ and determine the phase diagram in the T-μ plane. Our method is applicable to any number of Wilson or staggered quarks. As a direct test we showed that for $\mathrm{Im}(\mu)\neq 0$ 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 μ-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 μ_E is too large to be studied at RHIC or 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. More work is needed to get the final values by extrapolating in the R-algorithm and to the thermodynamic, chiral and continuum limits. The details of the presented results can be found in [22].

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