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Lattice determination of the critical point of QCD at finite T and μ

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Abstract: Based on universal arguments it is believed that there is a critical point (E) in QCD on the temperature (T) versus chemical potential (μ) plane, which is of extreme importance for heavy-ion experiments. Using finite size scaling and a recently proposed lattice method to study QCD at finite μ we determine the location of E in QCD with $n_f = 2 + 1$ dynamical staggered quarks with semi-realistic masses on $L_t = 4$ lattices. Our result is $T_E = 160 \pm 3.5\,\mathrm{MeV}$ and $\mu_E = 725 \pm 35\,\mathrm{MeV}$. For the critical temperature at $\mu = 0$ we obtained $T_c = 172 \pm 3\,\mathrm{MeV}$.

Keywords: Lattice Gauge Field Theories, Lattice QCD, Thermal Field Theory.

Contents

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 (for a clear introduction see [1]). QCD is asymptotically free, thus its high T and high density phases are dominated by partons (quarks and gluons) as degrees of freedom rather than hadrons. In this quark-gluon plasma (QGP) phase the symmetries of QCD are restored. In addition, recently a particularly interesting, rich phase structure has been conjectured for QCD at finite T and μ [2, 3].

Extensive experimental work has been done with heavy ion collisions at CERN and Brookhaven to explore the μ-T phase diagram. 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 open question, whether a critical point exists on the μ-T plane, and particularly how to predict theoretically its location [3, 4].

Let us discuss first the $\mu = 0$ case. Universal arguments [5] and lattice simulations [6] 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 an analytical crossover. Note, that observables change rapidly during a crossover, but no singularities appear (we will use the expression "transition" if we do not want to specify whether we deal with a phase transition or a crossover). This means that 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 [7] that m_s^c is about half of the physical m_s. Thus, in the real world we probably have a crossover. (Clearly, more work is needed to approach the chiral and continuum limits. Note, that the puzzle due to an unexpected strengthening observed [8] for the $n_f = 2$ Wilson action with intermediate $m_{u,d}$ was resolved by using an improved action [9].)

JHEP03(2002)014

Returning to a non-vanishing μ, one realizes that arguments based on a variety of models (see e.g. [10, 2, 3]) 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 [3]. At this point the phase transition is of second order and long wavelength fluctuations appear, which results in characteristic experimental consequences, similar to critical opalescence. Passing close enough to (μ_E,T_E) one expects simultaneous appearance of signatures (e.g. freeze-out type behavior of observables constructed from the multiplicity and transverse momenta of charged pions), which exhibit nonmonotonic dependence on the control parameters [11], since one can miss the critical point on either of two sides.

The location of this critical point is an unambiguous, non-perturbative prediction of the QCD lagrangian. Unfortunately, no *ab initio*, lattice analysis based on QCD was done to locate the endpoint. Crude models with $m_s = \infty$ were used (e.g. [3]) suggesting that $\mu_E \approx 700\,\mathrm{MeV}$, which should be smaller for finite m_s. The result is sensitive to m_s, thus for realistic cases previous works could not predict the value of μ_E even to within a factor of 2-3. The goal of this exploratory work is to show how to locate the endpoint by a lattice QCD calculation. We use full QCD with dynamical $n_f = 2 + 1$ staggered quarks.

QCD at finite μ can be formulated on the lattice [12]; however, standard Monte-Carlo techniques can not be used at $\mu \neq 0$. The reason is that for non-vanishing real μ the functional measure — thus, the determinant of the euclidean Dirac operator — is complex. This fact spoils any Monte-Carlo technique based on importance sampling. Several suggestions were studied to solve the problem. Unfortunately, none of them was able to locate (μ_E,T_E).

In a recent paper we proposed a new method [13] to study lattice QCD at finite T and μ. The idea was to produce an ensemble of QCD configurations at $\mu = 0$ and at T_c. Then we determined the Boltzmann weights [14] of these configurations at $\mu \neq 0$ and at T lowered to the transition temperatures at this non-vanishing μ. Since transition configurations were reweighted to transition configurations a much better overlap was observed than by reweighting pure hadronic configurations to transition ones [15]. We illustrated the applicability of the method in $n_f = 4$ dynamical QCD. Using only $\mathcal{O}(10^3$-$10^4)$ configurations quite large μ could be reached and the transition line separating the hadronic phase and the QGP was given on the μ-T plane.

In this letter we generalize the above method to arbitrary number of staggered quarks. We apply it to the $n_f = 2 + 1$ case. We determine the volume (V) dependence of the Lee-Yang zeros of the partition function on the complex gauge coupling (β) plane. Based on this V dependence we determine the type of the transition as a function of μ. The endpoint μ_E is given by the value at which the crossover disappears and finite-V scaling predicts a first order phase transition. These finite T calculations are done on $L_t = 4$ lattices. In order to set the physical scale we determine the pion and rho masses (m_π, m_ρ), the string-tension (σ) and the Sommer [16] scale (R_0) at $T = 0$. Our quark masses are "semi-realistic": m_s is set about to its physical value, whereas $m_{u,d}$ are approximately four times as heavy as they are in the real world. Having determined the lattice spacing we transform our result to physical units and give T_c the location of (μ_E,T_E) and show the phase diagram separating the hadronic phase and the QGP.

Though this study performes a V$\rightarrow\infty$ extrapolation, larger volumes, larger L_t-s and smaller masses are also needed to give the final answer to (μ_E,T_E).

2. Staggered quarks at $\mu \neq 0$

The partition function of QCD with n_f degenerate staggered quarks (for an introduction see eg. [17]) is given by the functional integral of the bosonic action S_b at gauge coupling β over the link variables U, weighted by the determinant of the quark matrix M, which can be rewritten [13] as

$$\begin{aligned} Z(\beta, m, \mu) &= \int \mathcal{D}U \exp[-S_b(\beta, U)][\det M(m,\mu,U)]^{n_f/4} \\ &= \int \mathcal{D}U \exp[-S_b(\beta_w, U)][\det M(m,\mu_w,U)]^{n_f/4} \times \\ &\qquad \times \left\{ \exp[-S_b(\beta,U) + S_b(\beta_w,U)] \frac{[\det M(m,\mu,U)]^{n_f/4}}{[\det M(m,\mu_w,U)]^{n_f/4}} \right\}, \end{aligned} \tag{2.1}$$

where m is the quark mass, μ is the chemical potential of the quark. For non-degenerate masses one uses simply the product of several quark matrix determinants on the 1/4-th power. Standard importance sampling works and can be used to collect an ensemble of configurations at β_w and μ_w with $\mathrm{Re}(\mu_w) = 0$. It means we treat the terms in the curly bracket as an observable — which is measured on each independent configuration — and the rest as the measure. By simultaneously changing β and μ one can ensure that even the mismatched measure at β_w and μ_w samples the regions where the original integrand with β and μ is large. In practice the determinant is evaluated at some μ and a Ferrenberg-Swendsen reweighting [14] is performed for the gauge coupling β.

Due to the complex nature of $\det M(m,\mu,U)$ an additional problem arises, one should choose among the possible Riemann-leaves of the fractional power in eq. (2.1). This can be done by using the fact that at $\mu = \mu_w$ the ratio of the determinants is 1 and the ratio should be a continuous function of μ. However, the continuity can only be ensured if the analytical dependence of the determinant on μ is known (the determinant oscillates strongly with μ, so measuring it for several μ values is not satisfactory). This dependence can be given by the following way (the idea goes back to a method of [18]).

First gauge fix to $A_0 = 0$ on all but the last timeslice

$$M = \begin{pmatrix} B_0 & e^{\mu} & 0 & \dots & e^{-\mu}T^\dagger \\ -e^{-\mu} & B_1 & e^{\mu} & \dots & \\ 0 & -e^{-\mu} & B_2 & \dots & \\ \vdots & \vdots & \vdots & \ddots & \\ -e^{\mu}T & & & & \end{pmatrix}. \tag{2.2}$$

The B_i are $3L_s^3 \times 3L_s^3$ matrices containing the mass and spatial hopping terms (3 is the number of colors) and T contains the only remaining temporal links on the last timeslice. By multiplying the j-th column of M by $e^{-j\mu}$ and the j-th row by $e^{j\mu}$ and moving the leftmost column to the right one gets a matrix with the same determinant

$$\begin{pmatrix} 1 & 0 & \dots & e^{-L_t\mu}T^\dagger & B_0 \\ B_1 & 1 & \dots & 0 & -1 \\ \vdots & \vdots & \ddots & & \vdots \\ & & & 1 & 0 \\ & & & B_{L_t-1} & -e^{L_t\mu}T \end{pmatrix}. \tag{2.3}$$

We evaluate the determinant by Gauss-elimination. After $L_t - 2$ steps we get a $6L_s^3 \times 6L_s^3$ matrix

$$\begin{pmatrix} 1 + c_1 \cdot e^{-L_t\mu} & c_2 \\ c_3 + c_4 \cdot e^{-L_t\mu} & c_5 - e^{L_t\mu}T \end{pmatrix}, \tag{2.4}$$

where c_i are μ-independent matrices. It is straightforward to show that

$$\det M = e^{-3L_s^3 L_t\mu} \det(P - e^{L_t\mu}), \tag{2.5}$$

where

$$P = \begin{pmatrix} -c_1 & c_2 T^\dagger \\ c_3 c_1 - c_4 & (c_5 - c_3 c_2)T^\dagger \end{pmatrix}. \tag{2.6}$$

This is just the characteristic equation of P. To find the λ_i eigenvalues one needs $\mathcal{O}(L_s^9)$ operations, which gives the determinant as a function of μ and determines the ratio of the fractional powers in eq. (2.1) unambiguously

$$\det M(\mu) = e^{-3L_s^3 L_t\mu} \prod_{i=1}^{6L_s^3} (e^{L_t\mu} - \lambda_i). \tag{2.7}$$

Using eq. (2.1) with the determinant given by eq. (2.7) we can give the partition function for complex μ and β values. In the following we keep μ real and look for the zeros of the partition function on the complex β plane. These are the Lee-Yang zeros [19], whose V$\to\infty$ behavior tells the difference between a crossover and a first order phase transition. At a first order phase transition the free energy $\propto \log Z(\beta)$ is non-analytic. Clearly, a phase transition can appear only in the V$\to\infty$ limit, but not in a finite V. Nevertheless, the partition function has zeros at finite V, the Lee-Yang zeros, at "unphysical" complex values of the parameters, in our case at complex β. For a system with a first order phase transition these zeros approach the real axis in the V$\to\infty$ limit (detailed analyzes suggest $1/V$ scaling). This V$\to\infty$ limit generates the non-analyticity of the free energy. For a system with crossover the free energy is analytic, thus the zeros do not approach the real axis in the V$\to\infty$ limit. The Lee-Yang technique was successfully applied to determine the endpoint of the electroweak phase transition [20, 21].

$\mathrm{Re}(\mu)$	0.1	0.2	0.3	0.4
$\mathrm{Re}(\beta_0)$; $L_s = 4$	5.151(1)	5.141(1)	5.127(2)	5.121(5)
$10^2\,\mathrm{Im}(\beta_0)$	5.56(8)	5.50(9)	5.42(15)	5.56(38)
$\mathrm{Re}(\beta_0)$; $L_s = 6$	5.193(1)	5.174(1)	5.152(3)	5.143(7)
$10^2\,\mathrm{Im}(\beta_0)$	2.66(6)	2.54(9)	2.19(31)	1.82(39)
$\mathrm{Re}(\beta_0)$; $L_s = 8$	5.193(1)	5.172(1)	5.159(1)	5.140(1)
$10^2\,\mathrm{Im}(\beta_0)$	1.38(6)	1.32(17)	1.31(18)	0.48(7)
$\mathrm{Re}(\beta_0)$; $L_s \to \infty$	5.201(1)	5.178(1)	5.162(2)	5.143(2)
$10^2\,\mathrm{Im}(\beta_0)$	1.02(6)	1.12(11)	0.74(19)	−0.25(10)
β	m_π	m_ρ	R_0	$\sqrt{\sigma}$
5.208	0.393(2)	1.22(2)	1.87(3)	0.58(7)
5.164	0.393(2)	1.28(3)	1.76(5)	0.75(5)

Table 1: $T \neq 0$ and $T = 0$ results. The upper part is a Summary of the Lee-Yang zeros obtained at different chemical potentials, while the lower part shows the measured $T = 0$ observables for two β values.

3. $T \neq 0$ and $T = 0$ results for $n_f = 2 + 1$

Using the formulation described above we study $n_f = 2+1$ QCD at $T \neq 0$ on $L_t = 4$, $L_s = 4, 6, 8$ lattices and at $T = 0$ on $V = 10^3 \cdot 16$ lattices. $m_{u,d} = 0.025$ and $m_s = 0.2$ were chosen for the bare quark masses. We used the R algorithm of the MILC collaboration's code [22].

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. The results (listed in table 1) are from 14000, 3600 and 840 configurations on $L_s = 4, 6$ and 8 lattices, respectively. Figure 1 shows $\mathrm{Im}(\beta_0^\infty)$ as a function of μ enlarged around the endpoint μ_{end}. The picture is simple and reflects the physical expectations. For small μ-s the extrapolated $\mathrm{Im}(\beta_0^\infty)$ is inconsistent with a vanishing value, and the prediction is a crossover. Increasing μ the value of $\mathrm{Im}(\beta_0^\infty)$ decreases, thus the transition becomes consistent with a first order phase transition. (Note, that errors decrease close to the endpoint, and the $\mathrm{Im}(\beta_0^\infty)$ extrapolation, due to the relatively small volumes, slightly overshoots. Both phenomena were observed already in the electroweak case e.g. [21]). The statistical error was determined by a jackknife analysis using subsamples of the total $L_s = 4, 6$ and 8 partition functions. The systematic uncertainty, estimated from the overshooting, was added linearly to the statistical error. The dashed line of figure 1 shows the fit and leads to our primary result: $\mu_{\mathrm{end}} = 0.375(20)$.

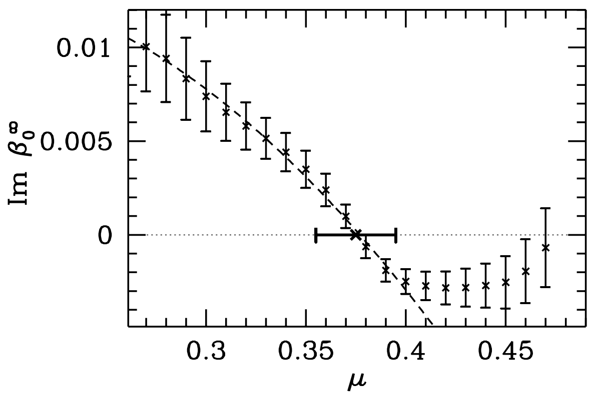

Figure 1: $\mathrm{Im}(\beta_0^\infty)$ as a function of the chemical potential.

Table 1 contains also the $T = 0$ results. To set the physical scale we used a weighted average of R_0 (1/403 MeV), m_ρ (770 MeV) and $\sqrt{\sigma}$ (440 MeV), obtained in lattice units by different fitting procedures. It is important to note, that (including systematic errors due to finite V) we have $(R_0 \cdot m_\pi) = 0.73(6)$, which is at least twice as large as its physical value. Thus our $m_{u,d}$ is at least four times larger than it should be.

Let us estimate the applicability of the method approaching the chiral and continuum limits. In the present analysis the evaluation of the eigenvalues was somewhat less costly than the production of the configurations. For physical $m_{u,d}$ the latter would need an additional factor of $\mathcal{O}(50)$ (the former remains the same). Thus, for physical masses at least upto V=$4{\cdot}12^3$ the cost of the eigenvalue determination is subdominant. Extending the analysis to this volume reduces the error on μ_{end} to a level, which is not even needed (uncertainties due to finite lattice spacing could be more important). Since for finer lattices the eigenvalue evaluation goes with L_s^9 and the configuration production at least with L_s^9 the eigenvalue evaluation remains subdominant. At physical masses μ_{end} is probably closer to the $\mu = 0$ axis (for recent lattice works see [7]). Thus, the overlap between $\mu = 0$ and $\mu \neq 0$ configurations is even better. It means less statistic might be enough to apply eq. (2.1) than it was used in this work. Note, that the quark masses of the present work are half of those used in ref. [13]; however, in both cases it was possible to reweight in μ far beyond $m_\pi/2$ (the typical premature onset μ value of the Glasgow method [15]). Thus, we expect that our method does not suffer from this type of onset problem when approaching the chiral limit.

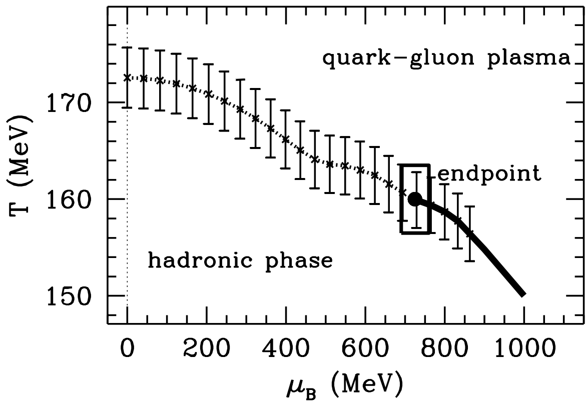

Figure 2: The phase diagram in physical units. Direct results are with errorbars. Dotted line illustrates the crossover, solid line the first order phase transition. The small box shows the uncertainties of the endpoint.

Figure 2 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 $\mu_B = 0$ we got $T_c = 172 \pm 3$ MeV.

4. Conclusions, outlook

We used a recently proposed method [13] and studied the μ-T phase diagram of QCD with dynamical $n_f = 2 + 1$ quarks. We presented an *ab initio* technique to determine the location of the endpoint. Using the above method we obtained $T_E = 160{\pm}3.5$ MeV for the temperature and $\mu_E = 725{\pm}35$ MeV for the baryonic chemical potential of the endpoint. This result was based on the V$\to\infty$ behavior of the Lee-Yang zeros of the partition function. We used $L_t = 4$ and our quark masses were “semi-realistic” (m_s was set to about its physical value, whereas $m_{u,d}$ were four times heavier than in the real world). Though μ_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.

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JHEP03(2002)014

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