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Critical point of QCD at finite T and μ, lattice results for physical quark masses

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Abstract: A critical point (E) is expected in QCD on the temperature (T) versus baryonic chemical potential (μ) plane. Using a recently proposed lattice method for $\mu \neq 0$ we study dynamical QCD with n_f=2+1 staggered quarks of physical masses on $L_t = 4$ lattices. Our result for the critical point is $T_E = 162 \pm 2\,\mathrm{MeV}$ and $\mu_E = 360 \pm 40\,\mathrm{MeV}$. For the critical temperature at $\mu = 0$ we obtained $T_c = 164 \pm 2\,\mathrm{MeV}$. This work extends our previous study [8] by two means. It decreases the light quark masses ($m_{u,d}$) by a factor of three down to their physical values. Furthermore, in order to approach the thermodynamical limit we increase our largest volume by a factor of three. As expected, decreasing $m_{u,d}$ decreased μ_E. Note, that the continuum extrapolation is still missing.

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

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Contents

1. Introduction

QCD is an asymptotically free theory, thus its high temperature and high density phases are dominated by partons (quarks and gluons) as degrees of freedom rather than hadrons. These phases play an important role in the particle physics of the early universe, of neutron stars and of heavy ion collisions (for a clear theoretical introduction and a review see [1, 2]).

Extensive experimental work has been done with heavy ion collisions at GSI, CERN and Brookhaven to study the strong interactions at high temperatures and non-vanishing baryon densities (the latter correspond to non-vanishing baryonic chemical potentials) and to explore the μ-T phase diagram. It is a long-standing open question, whether a critical point (E) exists on the μ-T plane, and particularly how to predict theoretically its location [3, 4]. At this point E 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. The observables exhibit non-monotonic dependence on the control parameters [5], 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, until recently no *ab initio*, lattice analysis based on QCD was done to locate the endpoint. Models with infinitely large strange quark mass (m_s=∞) were used (e.g. [3]), suggesting that $\mu_E \approx 700\,\text{MeV}$. The result is sensitive to the strange quark mass (μ_E should be smaller for smaller m_s). For realistic cases these techniques can not predict the value of μ_E even to within a factor of 2-3.

Lattice QCD at non-vanishing baryon density should, in principle, give an unambiguous answer. Though QCD at finite μ can be formulated on the lattice [6], 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 earlier to solve the problem. Unfortunately, none of them was able to give the phase line or locate (μ_E,T_E). About two years ago new techniques appeared, with which moderate chemical potentials could be reached on the lattice.

In two recent papers we proposed a new method [7, 8] to study lattice QCD at finite T and μ. The idea was to produce an ensemble of QCD configurations at μ=0 and at the corresponding transition temperature T_c (or at any other physically motivated point for which importance sampling works). Then we determined the Boltzmann weights [9] of these configurations at $\mu \neq 0$ and at T lowered to the transition temperatures at this non-vanishing μ. An ensemble of configurations at a transition point was reweighted to an ensemble of configurations at another transition point. With this technique a much better overlap was observed than by reweighting pure hadronic ensemble to a transition one [10]. We illustrated the applicability of the method in n_f=4 dynamical QCD [7] and in n_f=2+1 dynamical QCD [8]. The phase line with the critical end-point [8] and the equation of state [11, 12] were determined.

A less CPU demanding, truncated version of the overlap-improving multi-parameter reweighting was also applied using an improved lattice action. The approach can be summarized as follows. Instead of evaluating the Boltzmann weights exactly one can expand it in the chemical potential and use the first terms of the expansion. This modified technique was also able to give the phase diagram [13] and the equation of state [14] (estimates based on derivative extrapolation for the chiral endpoint was also reported in conference proceedings [15, 16]). The success of the overlap-improving multi-parameter reweighting was analyzed in ref. [17].

A completely independent method is based on the the fact that at imaginary chemical potential importance sampling works. The result on the phase digram can be analytically continued to real chemical potentials. This technique gave the phase line both in n_f=2 [18] and in n_f=4 [19], which are consistent with the results of the overlap-improving multi-parameter reweighting method [7, 8, 13]. Analytic continuation was also used to estimate the location of the critical endpoint [20] for n_f=3.

Recently several other new techniques were suggested (see e.g. [21, 22, 23]), which will be most probably tested in the near future. The recent developments of lattice QCD at non-vanishing chemical potentials are reviewed by refs. [24].

In this paper we use our original suggestion [7, 8] and evaluate the reweighting Boltzmann factors exactly. We determine the volume (V) dependence of the zeros of the partition function on the complex gauge coupling (β) plane. Based on this volume 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 volume 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, kaon and rho masses (m_π, m_K, m_ρ), and the Sommer [25] scale (R_0) at T=0. Our quark masses are realistic, the strange quark mass and the light quark masses are set about to their physical values. 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.

The present work is a significant improvement on our previous analysis by two means. We increased the physical volume by a factor of three and decreased the light quark masses by a factor of three, down to their physical values. Due to these improvements the computational effort of the present work was 140 times larger than that of the previous analysis [8].

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As expected, decreasing the light quark masses resulted in a smaller μ_E. Increasing the volumes did not influence the results, which indicates the reliability of the finite volume analysis. In order to give the final answer to (μ_E,T_E) the most important step remained is the continuum extrapolation. Note, however, that for the present physical problem decreasing the lattice spacing by a factor of 2 increases the CPU costs by approximately three orders of magnitude.

The remaining part of the paper is organized as follows. In section 2 we summarize the overlap-improving multi-parameter reweighting technique and the method of the Lee-Yang zeros, which can be used to separate the crossover and first order transition regions. Section 3 contains the details of the T≠0 and T=0 simulations. Those who are not interested in the lattice details could directly move to section 4, in which we present our results and conclude.

2. Overlap-improving multi-parameter reweighting at $\mu \neq 0$

The partition function of lattice QCD with n_f degenerate staggered quarks (for an introduction see e.g. [26]) 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 [7] as

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

where m is the quark mass, μ is the quark chemical potential and n_f is the number of flavours. 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 m_w, β_w and μ_w (with e.g. Re(μ_w)=0 or non-vanishing isospin chemical potential). 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 several parameters e.g. 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 [9] is performed for the gauge coupling β. The fractional power in eq. (2.1) can be taken by using the fact that at $\mu = \mu_w$ the ratio of the determinants is 1 and the ratio is a continuous function of the chemical potential. The details of the determinant calculation can be found in ref. [8].

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 [27]. Their V→ ∞ 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 Lee-Yang zeros at finite V. These are at "unphysical" complex values of the parameters, in our case at complex β-s. For a system with a first order phase transition these zeros approach the real axis in the V$\to\infty$ limit (the finite volume analysis of first order transitions suggests a $1/V$ scaling; see e.g. [28]). 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.

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

Using the formulation described above we study 2+1 flavour QCD at $T\neq 0$ on $L_t=4$, $L_s=6,8,10,12$ lattices with $m_{u,d}=0.0092$ and $m_s=0.25$ as bare quark masses. Note, that these mass parameters approximately correspond to their physical values. At $T=0$ we use $12^3\cdot 24$ lattices. Three different couplings (β=5.090, 5.160, 5.190) are studied in order to determine the non-perturbative β-function. Chiral extrapolation in the light quark masses at T=0 are done by using three different mass parameters ($m_{u,d}$=0.02, 0.04, 0.06). For each parameter set 3000 configurations were generated. For generating the field configurations the R algorithm is applied. The microcanonical stepsize is always set to half of the light quark mass. We use a modified version [29] of the MILC collaboration's code [30].

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 calculated by a $\beta_0(V)=\beta_0^\infty+\zeta/V$ extrapolation. The results (listed in table 1) are obtained by generating 100,000; 100,000; 100,000 and 150,000 configurations on our L_s=6,8,10 and 12 lattices, respectively. The determinant calculation was carried out after every 50 trajectories. Thus our results are based on a few thousand independent configurations.

Figure 1 shows Im(β_0^∞) 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 Im(β_0^∞) is inconsistent with a vanishing value, and the prediction is a crossover. Increasing μ the value of Im(β_0^∞) decreases, thus the transition becomes consistent with a first order phase transition. The statistical error was determined by a jackknife analysis using subsamples of the total L_s=6,8,10 and 12 partition functions. Our primary result in lattice units is $\mu_{end}=0.1825(75)$.

Table 1 contains also the $T=0$ results. To set the physical scale we used an average obtained from R_0 (0.5 fm) and m_ρ (770 MeV). Note, that these two quantities give somewhat different scales (the difference is fairly small, approximately 10-15%). This difference is expected to dissappear when one approaches the continuum limit with physical quark masses.[1]

Setting the scale leads to the final results of the analysis. As we already discussed, the quark masses, used to determine the endpoint, correspond approximately to their physical values. The pion to rho mass ratio, extrapolated to our $T\neq 0$ parameters, is 0.188(2) (its

[1]Note, that this difference is smaller than the difference in our previous analysis [8]. This improvement is due to the choice of the physical light quark masses.

Re(μ)	0.04	0.08	0.12	0.16	20
Re(β_0); $L_s = 6$	5.1863(9)	5.1839(9)	5.1800(9)	5.1749(11)	5.1713(14)
10^2Im(β_0)	2.39(6)	2.39(6)	2.41(8)	2.41(13)	2.26(22)
Re(β_0); $L_s = 8$	5.1886(4)	5.1858(5)	5.1811(5)	5.1753(7)	5.1710(16)
10^2 Im(β_0)	1.32(2)	1.33(3)	1.33(3)	1.28(5)	0.98(12)
Re(β_0); $L_s = 10$	5.1892(3)	5.1865(3)	5.1821(3)	5.1758(8)	5.1751(11)
10^3 Im(β_0)	7.27(14)	7.26(15)	7.33(22)	6.44(74)	5.29(76)
Re(β_0); $L_s = 12$	5.1888(2)	5.1861(2)	5.1817(3)	5.1768(4)	5.1739(6)
10^3 Im(β_0)	4.95(12)	4.95(13)	4.88(20)	4.16(71)	2.07(74)
Re(β_0);$L_s \to \infty$	5.1893(3)	5.1866(3)	5.1822(3)	5.1769(5)	5.1745(6)
10^3 Im(β_0)	2.12(14)	2.12(16)	2.14(23)	1.77(65)	-0.39(77)
β	$m_{u,d}$	m_π	m_K	m_ρ	R_0
5.09	0.02	0.3555(1)	0.8948(2)	1.361(9)	1.58(2)
5.09	0.04	0.4978(1)	0.9235(1)	1.391(4)	1.58(1)
5.09	0.06	0.6044(1)	0.9511(1)	1.423(4)	1.57(10)
5.16	0.02	0.3630(2)	0.9061(3)	1.306(10)	1.73(3)
5.16	0.04	0.5063(2)	0.9335(2)	1.344(8)	1.67(1)
5.16	0.06	0.6129(1)	0.9603(1)	1.389(4)	1.64(1)
5.19	0.02	0.3674(1)	0.9122(3)	1.287(8)	1.77(2)
5.19	0.04	0.5063(1)	0.9337(2)	1.325(6)	1.72(1)
5.19	0.06	0.6130(1)	0.9604(1)	1.366(2)	1.70(1)

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 for $m_{u,d}$=0.0092 and m_s=0.25. We indicate by 6,8,10,12 and ∞ the spatial extensions — and their extrapolation — of our $L_t = 4$ lattices. The lower part shows the measured $T = 0$ observables for three β and three $m_{u,d}$ values at m_s=0.25 on $12^3 \cdot 24$ lattices.

physical value is 0.179), whereas the pion to K mass ratio in the same limit is 0.267(1) (its physical value is 0.277).

Along the transition line β decreases, thus the lattice spacing increases. During the reweighting procedure we did not change the lattice quark masses, thus the quark masses changed in physical units. As a consequence, the transition line slightly deviates from the line of constant physics. We corrected for this effect by using our previous results at larger m_{ud} [8] and by following the observation that transition lines for slightly different quark masses are practically parallel (see [11, 12]). We can expand the transition temperature ($T_c(\mu, ma)$) linearly in the mass parameter:

$$T_c(\mu, ma) = T_c(\mu, m_1 a) + \frac{T_c(\mu, m_2 a) - T_c(\mu, m_1 a)}{m_2 a - m_1 a} \cdot (ma - m_1 a)\,, \tag{3.1}$$

where $m_1 a$ and $m_2 a$ are the mass parameters used in this paper and in ref. [8] while $T_c(\mu, m_2 a)$ and $T_c(\mu, m_1 a)$ are the corresponding μ dependent transition temperatures. Using the fact that along the transition line the lattice spacing is $a = 1/(L_t T_c)$, one can solve the above equation for $T_c(\mu, m)$ at a fixed physical m.

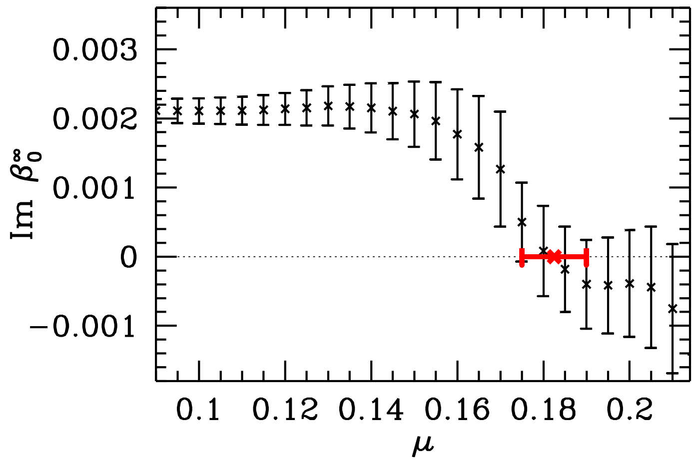

Figure 1: $\mathrm{Im}(\beta_0^\infty)$ as a function of the chemical potential.

Let us estimate the applicability of the method approaching the continuum limit. In the present analysis with physical quark masses the evaluation of the eigenvalues was somewhat less costly than the production of the configurations. Extending the analysis to even larger volumes, approximately upto $4{\cdot}16^3$, the eigenvalue determination remains subdominant. Using these larger volumes reduces the error on μ_{end} to a level, which is not even needed (uncertainties due to finite lattice spacing are more important). For finer lattices the eigenvalue evaluation goes with L_s^9 and the configuration production goes at least with L_s^9. According to numerical estimates [11, 12, 17] the applicability range of the overlap-improving multi-parameter reweighting technique, along the transition line, scales with $\mu \propto V^\gamma$ with $\gamma \approx 1/3$. (Note, that the systematic study of the lattice spacing dependence of γ has not been performed yet.) In the scaling region the chemical potential of the endpoint is constant in physical units. It scales with $V^{0.25}$ in lattice units for fixed physical volumes. Taking into account the marginal difference between $\gamma \approx 1/3$ and 0.25, one concludes that the determinant evaluation remains subdominant and even with the present technique one might successfully approach smaller lattice spacings.

4. Results and conclusions

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 transition temperature at vanishing baryonic chemical potential is T_c=164±2 MeV. Note, that this value is somewhat smaller than our previous result (T_c=172±3 MeV of ref. [8]). This is a known phenomenon: smaller quark mass results in smaller transition temperature (see e.g. [31]).

The curvature of the crossover line separating the QGP and the hadronic phases is given by $T/T_c = 1 - C\mu_B^2/T_c^2$ with C=0.0032(1). This value is somewhat smaller than our previous curvature [8] or other values in the literature [13, 15, 14, 18]. Note, that compared to other analyses, we took into account an additional effect which reduced the value of C.

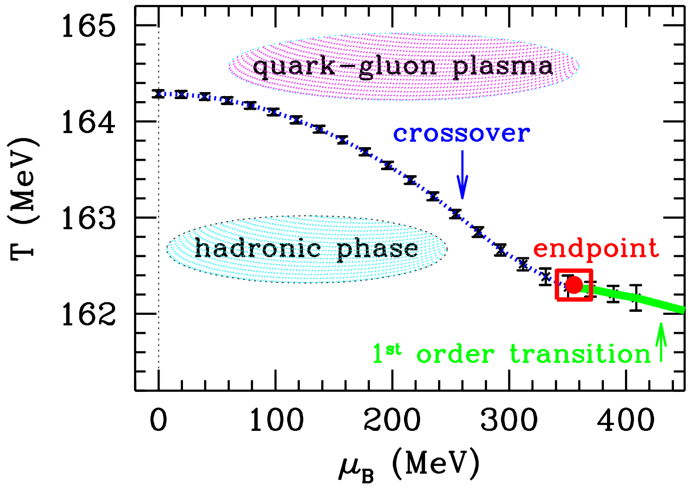

Figure 2: The phase diagram in physical units. Dotted line illustrates the crossover, solid line the first order phase transition. The small square shows the endpoint. The depicted errors originate from the reweighting procedure. Note, that an overall additional error of 1.3% comes from the error of the scale determination at T=0. Combining the two sources of uncertainties one obtains $T_E = 162 \pm 2\,\mathrm{MeV}$ and $\mu_E = 360 \pm 40\,\mathrm{MeV}$.

The small change of the mass parameter on the line of constant physics (caused by the change of the lattice spacing) slightly decreases the curvature.

The endpoint is at $T_E = 162 \pm 2\,\mathrm{MeV}$, $\mu_E = 360 \pm 40\,\mathrm{MeV}$. As expected, μ_E decreased as we decreased the light quark masses down to their physical values (at approximately three-times larger $m_{u,d}$ the critical point was at μ_E=720 MeV; see [8]).

The above result is a significant improvement on our previous analysis [8] by two means. We increased the physical volume by a factor of three and decreased the light quark masses by a factor of three. We carried out the whole analysis using four subsets of our volumes ($L_s = 6, 8, 10$, $L_s = 6, 8$, $L_s = 8, 10, 12$ and $L_s = 10, 12$) and found that the results changed only within their uncertainties. This fact indicates that the volumes of the present study are large enough and that the finite volume analysis is reliable. We do not expect finite size effects on μ_E. Clearly, more work is needed to get the final values. Most importantly one has to extrapolate to the continuum limit.

Acknowledgments

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