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

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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 ($\mu$) 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 $\mu$ 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 $T_E = 160 \pm 3.5$ MeV and $\mu_E = 725 \pm 35$ MeV. For the critical temperature at $\mu = 0$ we obtained $T_c = 172 \pm 3$ MeV.

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

QCD at finite $T$ and/or $\mu$ is of fundamental importance, since it describes relevant features of particle physics in the early universe, in neutron stars and in heavy ion collisions (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 $\mu$ [2, 3].

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

Let us discuss first the $\mu=0$ case. Universal arguments [3] 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 [4].)
Returning to a non-vanishing $\mu$, 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 $\mu$. Combining the $\mu = 0$ and large $\mu$ informations an interesting picture emerges on the $\mu$-$T$ plane. For the physical $m_s$ the first order phase transitions at large $\mu$ 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 $\mu_E$ 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 $(\mu_E, T_E)$ 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 $\mu_E \approx 700$ 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 $\mu_E$ 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 $\mu$ 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 $\mu$ 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 $(\mu_E, T_E)$.

In a recent paper we proposed a new method [13] to study lattice QCD at finite $T$ and $\mu$. 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 $\mu$. 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 $O(10^3-10^4)$ configurations quite large $\mu$ could be reached and the transition line separating the hadronic phase and the QGP was given on the $\mu$-$T$ 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 ($\beta$) plane. Based on this $V$ dependence we determine the type of the transition as a function of $\mu$. The endpoint $\mu_E$ 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 ($m_\pi, m_\rho$), the string-tension ($\sigma$) 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 $(\mu_E, T_E)$ and show the phase diagram separating the hadronic phase and the QGP.

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

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 $\beta$ over the link variables $U$, weighted by the determinant of the quark matrix $M$, which can be rewritten [13] as

$$Z(\beta, m, \mu) = \int DU \exp[-S_b(\beta, U)][\det M(m, \mu, U)]^{n_f/4}$$

$$= \int DU \exp[-S_b(\beta_w, U)][\det M(m, \mu_w, U)]^{n_f/4}$$

$$\left\{ \exp[-S_b(\beta, U) + S_b(\beta_w, U)]\frac{[\det M(m, \mu, U)]^{n_f/4}}{[\det M(m, \mu_w, U)]^{n_f/4}} \right\} ,$$

where $m$ is the quark mass, $\mu$ 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 $\beta_w$ and $\mu_w$ with $\text{Re}(\mu_w)=0$. 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 $\beta$ and $\mu$ one can ensure that even the mismatched measure at $\beta_w$ and $\mu_w$ samples the regions where the original integrand with $\beta$ and $\mu$ is large. In practice the determinant is evaluated at some $\mu$ and a Ferrenberg-Swendsen reweighting [14] is performed for the gauge coupling $\beta$.

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 $\mu$. However, the continuity can only be ensured if the analytical dependence of the determinant on $\mu$ is known (the determinant oscillates strongly with $\mu$, so measuring it for several $\mu$ values is not satisfactory). This dependence can be given by the following way (the idea goes back to a method of [15]).

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

$$M = \begin{pmatrix} 
B_0 & e^\mu & 0 & \ldots & e^{-\mu}T^+ \\
-e^{-\mu} & B_1 & e^\mu & \ldots \\
0 & -e^{-\mu} & B_2 & \ldots \\
\vdots & \vdots & \vdots & \ddots \\
-e^\mu T & & & & 
\end{pmatrix} .$$

(2.2)
The $B_t$ 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

$$
\begin{pmatrix}
1 & 0 & \ldots & e^{-Lt\mu}T & B_0 \\
B_1 & 1 & \ldots & 0 & -1 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
1 & 0 & \ldots \\
B_{Lt-1} & e^{Lt\mu}T
\end{pmatrix}
$$

(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

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

(2.4)

where $c_i$ are $\mu$-independent matrices. It is straightforward to show that

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

(2.5)

where

$$
P = \left(\begin{array}{cc}
-c_1 & c_2 T^\dagger \\
-c_3 c_1 - c_4 & (c_5 - c_3 c_2 ) T^\dagger
\end{array}\right).
$$

(2.6)

This is just the characteristic equation of $P$. To find the $\lambda_i$ eigenvalues one needs $O(L_t^8)$ operations, which gives the determinant as a function of $\mu$ and determines the ratio of the fractional powers in eq. (2.1) unambiguously

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

(2.7)

Using eq. (2.1) with the determinant given by eq. (2.7) we can give the partition function for complex $\mu$ and $\beta$ values. In the following we keep $\mu$ real and look for the zeros of the partition function on the complex $\beta$ 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 $\beta$. 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].

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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 \[22\].

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

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 $\beta$ values.

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. 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 $\text{Im}(\beta_0^\infty)$ as a function of $\mu$ enlarged around the endpoint $\mu_{end}$. The picture is simple and reflects the physical expectations. For small $\mu$-s the extrapolated $\text{Im}(\beta_0^\infty)$ is inconsistent with a vanishing value, and the prediction is a crossover. Increasing $\mu$ the value of $\text{Im}(\beta_0^\infty)$ decreases, thus the transition becomes consistent with a first order phase transition. (Note, that errors decrease close to the endpoint, and the $\text{Im}(\beta_0^\infty)$ 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: $\mu_{\text{end}} = 0.375(20)$.

Table 1 contains also the $T = 0$ results. To set the physical scale we used a weighted
average of $R_0$ (1/403 MeV), $m_\rho$ (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 $O(50)$ (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 $\mu_{\text{end}}$ to a level, which is
not even needed (uncertainties due to finite lattice spacing could be more important). Since for finer lattices the eigen-
value evaluation goes with $L_s^6$ and the configuration production at least with $L_s^9$ the eigen-
value evaluation remains subdominant. At physical masses $\mu_{\text{end}}$ is probably closer to the
$\mu = 0$ axis (for recent lattice works see [9]). 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 $\mu$ far beyond
$m_\pi/2$ (the typical premature onset $\mu$ 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 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 got $T_c$
$= 172 \pm 3$ MeV.

4. Conclusions, outlook.

We used a recently proposed method [13] and studied the $\mu$-$T$ 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 $\mu_E$ 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 $T_c=172\pm3$ 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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References

[1] F. Wilczek, hep-ph/0003183.
[2] M. Alford, K. Rajagopal and F. Wilczek, Phys. Lett. B422 (1998) 247, Nucl. Phys. B537 (1999) 443; R. Rapp, T. Schäfer, E.V. Shuryak and M. Velkovsky, Phys. Rev. Lett. 81 (1998) 53; for a recent review with references see K. Rajagopal and F. Wilczek, hep-ph/0011333.
[3] M. Halasz et al. Phys. Rev. D58 (1998) 096007; J. Berges and K. Rajagopal, Nucl. Phys. B538 (1999) 215. M. Stephanov, K. Rajagopal and E. Shuryak, Phys. Rev. Lett. 81 (1998) 4816.
[4] T.M. Schwarz, S.P. Klevansky and G. Papp, Phys. Rev. C60 (1999) 055205.
[5] R. Pisarski and F. Wilczek, Phys. Rev. D29 (1984) 338; F. Wilczek, Int. J. Mod. Phys. A7 (1992) 3911; K. Rajagopal and F. Wilczek, Nucl. Phys. B399 (1993) 395.
[6] For recent reviews see: A. Ukawa, Nucl. Phys. Proc. Suppl. 53 (1997) 106; E. Laerman, ibid. 63 (1998) 114; F. Karsch, ibid. 83 (2000) 14; S. Ejiri, ibid. 94 (2001) 19.
[7] F.K. Brown, Phys. Rev. Lett. 65 (1990) 2491; S. Aoki et al., Nucl. Phys. Proc. Suppl. 73 (1999) 459.
[8] C. Bernard et al., Phys. Rev. D49 (1994) 3574; T. Blum et al., ibid. D50 (1994) 3377; Y. Iwasaki et al., ibid. D54 (1996) 7010.
[9] Y. Iwasaki et al., Phys. Rev. Lett. 78 (1997) 179; A. Ali Khan et al., Phys. Rev. D63 (2000) 034502.
[10] A. Barducci et al., Phys. Lett. B231 (1989) 463; Phys. Rev. D41 (1990) 1610; ibid. D49 (1994) 426; S.P. Klevansky, Rev. Mod. Phys. 64 (1992) 649; M. Stephanov, Phys. Rev. Lett. 76 (1996) 4472.
[11] M. Stephanov, K. Rajagopal and E. Shuryak, Phys. Rev. D60 (1999) 114028.
[12] P. Hasenfratz and F. Karsch, Phys. Lett. B125 (1983) 308; J. Kogut et al., Nucl. Phys. B225 (1983) 93.
[13] Z. Fodor and S.D. Katz, hep-lat/0104001.
[14] A.M. Ferrenberg and R.H. Swendsen, Phys. Rev. Lett. 63 (1989) 1195; ibid. 61 (1988) 2635.
[15] I.M. Barbour et al., Nucl. Phys. B (Proc. Suppl.) 60A (1998) 220.
[16] R. Sommer, Nucl. Phys. B411 (1994) 839.

[17] I. Montvay and G. Münster, Quantum fields on a lattice, Cambridge, UK, University Press (1994).

[18] D. Toussaint, Nucl. Phys. Proc. Suppl. 17 (1990) 248.

[19] C.N. Yang and T.D. Lee, Phys. Rev. 87 (1952) 404.

[20] F. Karsch et al. Nucl. Phys. B (Proc. Suppl.) 53 (1997) 623; M. Gürtler et al., Phys. Rev. D56 (1997) 3888.

[21] F. Csikor, Z. Fodor and J. Heitger, Phys. Rev. Lett. 82 (1999) 21; Y. Aoki et al. Phys. Rev. D60 (1999) 013001.

[22] MILC collaboration’s public lattice gauge theory code. See http://physics.indiana.edu/~sg/milc.html.