The QCD phase diagram at nonzero quark density

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ABSTRACT: We determine the phase diagram of QCD on the $\mu - T$ plane for small to moderate chemical potentials. Two transition lines are defined with two quantities, the chiral condensate and the strange quark number susceptibility. The calculations are carried out on $N_t = 6, 8$ and $10$ lattices generated with a Symanzik improved gauge and stout-link improved 2+1 flavor staggered fermion action using physical quark masses. After carrying out the continuum extrapolation we find that both quantities result in a similar curvature of the transition line. Furthermore, our results indicate that in leading order the width of the transition region remains essentially the same as the chemical potential is increased.

KEYWORDS: Lattice QCD Thermodynamics, Sign problem.

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1. Introduction

The understanding of the phase diagram of QCD is of utmost importance and has attracted much attention, both experimental and theoretical. Experimental results are coming from cosmology and heavy ion collisions. Recently, in a collision of gold nuclei at the Relativistic Heavy Ion Collider (RHIC), a temperature beyond 200 MeV was reached [1], which indicates that the quark-gluon plasma has been created. Furthermore, the density of the system can be varied by tuning the center of mass energy $\sqrt{s_{NN}}$. While most of the ongoing experiments like those at LHC or RHIC concentrate on achieving very high energies and thus small chemical potentials, there are projects that aim for regions of the phase diagram with larger densities (RHIC II, Facility for Antiproton and Ion Research (FAIR)). In these latter experiments an important objective is to identify the critical endpoint, e.g., by searching for critical opalescence. Designing these next generation experiments can benefit greatly from developing theoretical understanding of the phase diagram.

Our theoretical knowledge about the phase diagram of QCD is mostly limited to the zero chemical potential ($\mu = 0$) axis and obtained by the use of lattice QCD. The main reason that full results for $\mu > 0$ are not available is the infamous sign problem which spoils any lattice technique based on importance sampling. There are various scenarios for the $\mu > 0$ region of the phase diagram, among which two are illustrated in Figure 1.

The transition at $\mu = 0$ is a crossover [2] and we expect that the transition temperature decreases as we increase $\mu$. Besides the actual value of the curvature of the transition line a particularly interesting question is whether the transition becomes weaker or stronger as $\mu$ grows. A strengthening of the transition could lead to the existence of a critical point, where the crossover transforms into a true phase transition (see left side of Figure 1). Another possibility is that the transition weakens with increasing $\mu$ (see right side of Figure 1). The
existence of the critical point would not be ruled out by such a scenario but would require non-monotonic behavior [3].

At zero chemical potential lattice calculations provide reliable and accurate results [4–9]. Much more difficult is the situation at nonzero chemical potential. Simulations at non-vanishing chemical potential are burdened by the sign (complex action) problem: the fermion determinant here becomes complex, and as a result makes Monte-Carlo methods based on importance sampling impossible. Recently several methods were developed to access the region of small chemical potentials. They are all based on simulations at zero or purely imaginary chemical potentials where the sign problem is absent. The first possibility is the reweighting of the generated configurations [10–14]. The weight factors can also be approximated by a Taylor expansion in \( \mu \) [15–19]. Further possibilities are an analytic continuation from imaginary \( \mu \) [20–27], or using the canonical ensemble [28–30]. The above studies were carried out on coarse lattices and in most cases with non-physical quark masses. We emphasize that to have a full result, the use of physical quark masses and a reliable continuum extrapolation are essential. In this paper we determine the transition temperature \( T_c(\mu) \) as a function of the chemical potential through a Taylor-expansion technique. The first term of this expansion is zero due to the symmetry \( \mathcal{Z}(\mu) = \mathcal{Z}(-\mu) \) of the partition function. Therefore the first nonvanishing contribution comes from the second order, which is related to the curvature of the transition line.

2. Definition of the curvature

Let us parameterize the transition line in the vicinity of the vertical \( \mu = 0 \) axis as

\[
T_c(\mu^2) = T_c \left( 1 - \kappa \cdot \mu^2 / T_c^2 \right)
\]  

(2.1)
with $T_c$ being short for $T_c(0)$. This implies that the curvature can be written as

$$\kappa = -T_c \left. \frac{dT_c(\mu^2)}{d(\mu^2)} \right|_{\mu=0} \tag{2.2}$$

where (and also in the following) $\mu$ refers to the baryonic chemical potential ($\mu \equiv \mu_B = 3\mu_{u,d}$), where $\mu_{u,d}$ is the quark chemical potential assigned to the light quarks. Thus one has to measure $T_c$ as a function of $\mu$ for small chemical potentials. To this end we use a definition of $T_c$ which is most suitable for determining the curvature.

Let us consider a quantity $\phi(T,\mu^2)$ that is monotonic in $T$ in the transition region, and fulfills the following constraints:

$$\lim_{T \to 0} \frac{\partial}{\partial \mu^2} \phi(T,\mu^2) = 0, \quad \lim_{T \to \infty} \frac{\partial}{\partial \mu^2} \phi(T,\mu^2) = 0 \tag{2.3}$$

that is to say, $\phi$ does not depend on the chemical potential in the limiting cases $T \to 0$ and $T \to \infty$. For any fixed $\mu$ we can define a transition temperature $T_c(\mu^2)$ as the temperature at which $\phi(T,\mu^2)$ takes the predefined constant value $C$:

$$\phi(T,\mu^2)|_{T=T_c(\mu^2)} = C. \tag{2.4}$$

We will choose a $C$ that corresponds to the inflection point of $\phi(T,0)$. (Note that $T_c$ can also be defined as the location of the maximum or inflection point of some observable. At non-zero $\mu$ this turns out to be somewhat less advantageous since a fitting of the reweighted data is required.)

Now let us determine the curvature using this definition of $T_c(\mu^2)$. The total derivative of the observable $\phi(T,\mu^2)$ may be written as

$$d\phi = \left. \left( \frac{\partial \phi}{\partial T} \right) \right|_{\mu=0} \cdot dT + \left. \left( \frac{\partial \phi}{\partial (\mu^2)} \right) \right|_{\mu=0} \cdot d\mu^2 \tag{2.5}$$

Along the $T_c(\mu^2)$ line, $\phi$ is constant by definition, thus $d\phi = 0$. One obtains

$$\frac{dT_c}{d\mu^2} = - \left. \left( \frac{\partial \phi}{\partial (\mu^2)} \right) \right|_{\mu=0} / \left. \left( \frac{\partial \phi}{\partial T} \right) \right|_{\mu=0} \tag{2.6}$$

Thus, for every $C$ we can define a curvature. Since the $T_c(C)$ function is invertible for the whole $C$ range, we can also write (2.6) as a function of temperature, $R(T)$.

The function $R(T)$ is related to the distance that the $\phi(T)$ curve shifts along the $T$ axis as the chemical potential is varied. Given $\phi(T)$ and $R(T)$ at zero chemical potential, the shift for non-zero $\mu$ at leading order is $R(T) \cdot \mu^2$ (the curve moves to the left if $R(T)$ is negative and to the right otherwise). This behavior is illustrated in Figure 2. Using $R(T)$ we can define a temperature dependent curvature according to (2.2) as $\kappa(T) = -T_c \cdot R(T)$. The meaning of $\kappa(T)$ is again simple: it gives the curvature of the $\phi = \text{const}.$ curve which starts from $T$ at $\mu = 0$.

We use the value of $\kappa(T)$ at $T = T_c$ to define the curvature for a given observable. The shape of the $\kappa(T)$ function also has important consequences. The slope of $\kappa(T)$ around $T_c$ is related to the width of the transition as follows: if the slope is zero, i.e. $\kappa(T)$ is
constant around $T_c$, then all points shift the same amount along the $T$ axis when a small chemical potential is switched on. This means that to leading order in $\mu$ the shape of the $\phi(T)$ function (and thus, the width of the transition) does not change. If the slope is positive, then points with larger $T$ shift more than the ones with smaller $T$ resulting in a compression of points, i.e. a narrower transition. Similarly, a negative slope indicates a broadening of the transition.

All in all, the expression $\partial \kappa / \partial T$ is therefore related to the relative change in the width $W(\mu)$ of the transition as the chemical potential increases:

$$\frac{1}{W} \frac{\partial W}{\partial (\mu^2)} = - \frac{1}{T_c} \frac{\partial \kappa}{\partial T} \bigg|_{T = T_c}$$

where we assume that $W$ is proportional to the inverse slope of the quantity in question: $W \sim \left| (\partial \phi / \partial T)_{T=T_c} \right|^{-1}$.

The two observables we use are the renormalized chiral condensate $\phi = \langle \bar{\psi} \psi \rangle$ and the normalized strange quark number susceptibility $\phi = \langle \chi_s / T^2 \rangle$. As we show in section 4, both satisfy the constraints listed in (2.3). The derivative $\partial \phi / \partial T$ is determined numerically, using the $\mu = 0$ data as a function of the temperature. In order to calculate the derivative $\partial \phi / \partial (\mu^2)$ we need to measure more complicated operators; the technique for computing these is detailed in the next section.

3. Determination of the Taylor-coefficients

Let us consider the partition function of the staggered lattice formulation for $N_f$ fermion flavors in its usual form

$$Z = \int \mathcal{D}U e^{-S_g(U)} (\det M)^{N_f/4}$$

and denote the derivative with respect to $\mu_{u,d}$ by $'$. The derivatives of $Z$ are easily calculated to be $(\log Z)' = \langle n_{u,d} \rangle$ and $(\log Z)'' = \langle n_{u,d}^2 + n'_{u,d} \rangle - \langle n_{u,d} \rangle^2$, where the light quark number
density $n_{u,d}$ and its derivative with respect to $\mu_{u,d}$ are given by the following combinations:

$$n_{u,d} = \frac{N_f}{4} \text{Tr} \left( M^{-1} M' \right)$$

$$n'_{u,d} = \frac{N_f}{4} \text{Tr} \left( M^{-1} M'' - M^{-1} M' M^{-1} M' \right)$$

Using these definitions the second derivative of any (possibly explicitly $\mu$-dependent) observable can be straightforwardly determined. For the renormalized chiral condensate and the strange quark number susceptibility (see definition in section 4) one obtains:

$$\frac{\partial^2 \langle \bar{\psi} \psi \rangle}{\partial \mu_{u,d}^2} \bigg|_{\mu_{u,d}=0} = \langle \bar{\psi} \psi/(n_{u,d}^2 + n'_{u,d}) \rangle - \langle \bar{\psi} \psi \rangle \langle n_{u,d}^2 + n'_{u,d} \rangle + \langle 2 \bar{\psi} \psi' n_{u,d} + \bar{\psi} \psi'' \rangle$$

(3.2)

$$\frac{\partial^2 \langle \chi_s \rangle}{\partial \mu_{u,d}^2} \bigg|_{\mu_{u,d}=0} = \langle \chi_s (n_{u,d}^2 + n'_{u,d}) \rangle - \langle \chi_s \rangle \langle n_{u,d}^2 + n'_{u,d} \rangle - 2 \langle n_s n_{u,d} \rangle^2$$

(3.3)

where $n_s$ is the strange quark number density, defined similarly as $n_{u,d}$. Note that the additive renormalization of $\bar{\psi} \psi$ (see section 4.2) does not influence the derivative in question.

For the chiral condensate – being a $\mu$-dependent operator – the derivatives $\bar{\psi} \psi'$ and $\bar{\psi} \psi''$ of this explicit dependence are also present in (3.2). These terms were calculated numerically, using a purely imaginary chemical potential $\Delta \mu_i$. The value of $\Delta \mu_i$ was varied in the range $0.01 \ldots 0.0005$, and it was checked that the finite differences converge fast enough to the $\Delta \mu_i \to 0$ values and the error coming from this approximation is negligible compared to statistical errors. Taking into account these considerations $\Delta \mu_i = 0.001$ was used.

4. The $\mu$-dependence of the observables

We calculated the curvature of the transition line using the strange quark number susceptibility and the chiral condensate. The details of their renormalization and behavior are explained in this section.

4.1 The strange quark number susceptibility

The strange quark number susceptibility is defined as

$$\langle \chi_s \rangle = \frac{T}{V} \frac{\partial^2 \log Z}{\partial \mu_i^2}$$

(4.1)

This observable needs no renormalization, since it is connected to a conserved current. It is useful to study the combination $\langle \chi_s / T^2 \rangle$, since it obeys the conditions of (2.3). It is easy to see that at $T = 0$ one gets $\langle \chi_s / T^2 \rangle = 0$ and at $T \to \infty$ the normalized quark number susceptibility $\langle \chi_s / T^2 \rangle$ reaches its $\mu_{u,d}$ independent Stefan-Boltzmann limit of 1.

4.2 The chiral condensate

The chiral condensate can also be expressed as a derivative of the partition function:

$$\langle \bar{\psi} \psi \rangle = \frac{T}{V} \frac{\partial \log Z}{\partial m}$$

(4.2)
The renormalization of $\bar{\psi}\psi$ is a more delicate issue as compared to the situation with $\chi_s$. The free energy ($\log Z$) contains additive divergences in the cutoff. In order to carry out the proper renormalization of the condensate, these additive divergences have to be eliminated – this is done by subtracting the $T = 0$ contribution.

The multiplicative divergence due to the derivative with respect to the mass can be eliminated with a multiplication by the bare quark mass. Then, in order to have a dimensionless combination$^1$, the whole expression can be divided by the fourth power of some dimensionful mass scale, $Q^4$:

$$
\langle \bar{\psi}\psi_r \rangle = (\langle \bar{\psi}\psi \rangle - \langle \bar{\psi}\psi \rangle(T = 0)) \cdot m \cdot \frac{1}{Q^4}
$$

This way no divergent contributions remain: this is a meaningful quantity to study in the continuum limit.$^2$ In this work we use the $T = 0$ pion mass for the $Q$ normalization scale.

The final condition that has to be satisfied is that $\langle \bar{\psi}\psi_r \rangle$ should be independent of $\mu$ at $T = 0$ and $T \to \infty$. At $T = 0$ the partition function is independent of $\mu$ as long as $\mu$ is smaller than a $\mu_c$ critical value (the approximate baryon mass) and no baryons can be created from the vacuum. Only for $\mu > \mu_c$ does the partition function have a non-trivial $\mu$ dependence. Therefore all derivatives of $Z$ (thus $\langle \bar{\psi}\psi_r \rangle$) are independent of $\mu$ for $\mu < \mu_c$. The chemical potential regime covered in this paper lies in this region. In the Stefan-Boltzmann limit ($T \to \infty$) the $\mu$ independence is only satisfied in the sense $(\bar{\psi}\psi_r)^{-1} \partial/\partial \mu^2(\bar{\psi}\psi_r) \to 0$. Figure 4 demonstrates, however, that for temperatures above the transition region $\bar{\psi}\psi_r$ is already practically independent of $\mu$.

Figure 3 illustrates the behavior of $\langle \chi_s/T^2 \rangle$ and $\langle \bar{\psi}\psi_r \rangle$ as a function of the temperature, determined on $N_t = 10$ lattices.

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1 Note that a division by $T^4$ which would also render the condensate dimensionless, changes the temperature dependence and would lead to a non-monotonic $T$ dependence, which would be disadvantageous in the present context.

2 Note that this renormalization procedure leads to a somewhat unusual chiral condensate which vanishes at $T = 0$ and reaches a negative value at $T \to \infty$. A more conventional condensate which is positive at $T = 0$ and goes to zero at large temperatures can be obtained by a constant shift which is irrelevant for our present study.
5. Simulation setup

We used a Symanzik improved gauge and stout-link improved staggered fermionic lattice action in order to reduce taste violation [5]. The configurations were generated with an exact RHMC algorithm [31]. We determined the line of constant physics (LCP) using physical masses for the light quarks \( m_{u,d} \) as well as for the strange quark \( m_s \). The LCP was fixed by setting the ratios \( m_K/f_K \) and \( m_K/m_\pi \) to their physical values. We used three different lattice spacings \( N_t = 6, 8, 10 \) and aspect ratios \( N_s/N_t \) of 4 and 3. The scale was fixed by \( f_K \) and its unambiguity was checked by calculating \( m_{K^*}, f_\pi \) and \( r_0 \). The random noise estimator method was used to measure the operators detailed in section 3. We used 80 random vectors so that the error coming from the method and the statistical error are of the same extent. The details of the simulation setup can be found elsewhere [5, 32]. We used the gauge ensembles generated for a \( \mu = 0 \) study [5]. We also generated extra configurations for \( N_t = 8 \) and 10. The number of trajectories at each \( \beta, N_s \) and \( N_t \) is summarized in table 1. The autocorrelation times were below 10 trajectories in all cases. After confirming the absence of thermalization effects, we measured observables on every fifth trajectory. The measurements were performed on clusters equipped with graphics cards [33].

\[
\begin{array}{|c|c|c|}
\hline
N_s^3 \times N_t & \beta & \# \text{ of trajs.} \\ \hline
24^3 \times 6 & 3.4500 & 1750 \\ & 3.4950 & 2500 \\ & 3.5100 & 5200 \\ & 3.5250 & 5350 \\ & 3.5400 & 3440 \\ & 3.5550 & 3400 \\ & 3.5700 & 3350 \\ & 3.5850 & 4650 \\ & 3.6000 & 3600 \\ & 3.6450 & 3650 \\ & 3.5550 & 4550 \\ \hline
24^3 \times 8 & 3.6000 & 1800 \\ & 3.6250 & 2100 \\ & 3.6375 & 4050 \\ & 3.6500 & 3000 \\ & 3.6625 & 3150 \\ & 3.6750 & 3200 \\ & 3.6813 & 3200 \\ & 3.6875 & 14350 \\ & 3.7000 & 4050 \\ & 3.7125 & 850 \\ & 3.7250 & 800 \\ & 3.7500 & 2300 \\ & 3.7625 & 800 \\ & 3.7750 & 5050 \\ & 3.7875 & 4200 \\ & 3.8000 & 1600 \\ & 3.8125 & 2000 \\ & 3.8250 & 4850 \\ & 3.8375 & 4150 \\ & 3.8550 & 5950 \\ \hline
28^3 \times 10 & 3.6500 & 800 \\ & 3.6750 & 3350 \\ & 3.7000 & 800 \\ & 3.7125 & 800 \\ & 3.7500 & 2300 \\ & 3.7625 & 800 \\ & 3.7750 & 5050 \\ & 3.7875 & 4200 \\ & 3.8000 & 1600 \\ & 3.8125 & 2000 \\ & 3.8250 & 4850 \\ & 3.8375 & 4150 \\ & 3.8550 & 5950 \\ \hline
\end{array}
\]

Table 1: Number of trajectories for various lattice geometries.

6. Results

First we checked finite size effects by comparing our results at \( \beta = 3.555 \) obtained on \( 24^3 \times 6 \) and on \( 18^3 \times 6 \) lattices. This value of \( \beta \) corresponds to about 155 MeV, i.e. is near the pseudocritical temperature. The larger box is of physical size \( \sim 5 \) fm. We observe a good agreement as the results for \( \partial \phi/\partial (\mu^2) \) agree within statistical errors for both the chiral condensate \( \phi = \langle \bar{\psi} \psi \rangle \) and the strange quark number susceptibility \( \phi = \langle \chi_s/T^2 \rangle \). Figure 4 shows our \( N_t = 6 \) results for \( N_s = 24 \) and \( N_s = 18 \). Thus we conclude that finite size errors can be neglected at the present statistical accuracy.

Since the actual shape of the \( \kappa(T) \) function is unknown we carry out a Taylor expansion around \( T_c \) in the \( t = (T - T_c)/T_c \) dimensionless variable:

\[
\kappa(T) = \kappa(T_c) + c_0 \cdot t + c_1 \cdot t^2
\]

(6.1)
Figure 4: The derivative of our observables with respect to $\mu^2$ measured on $N_t = 6$ lattices. The $N_s = 24$ results (blue points) are checked at one temperature by $N_s = 18$ (red point). In the case of both observables a good agreement is observed, which indicates that finite size effects are small as compared to statistical errors.

For each lattice spacing (i.e. each $N_t$) we have several simulation points, corresponding to different temperatures. In order to fit all of our points at once, we allow a lattice spacing dependence for the constant and linear terms (having a lattice spacing dependence of the quadratic term is also possible, but it does not improve the quality of the fits). Therefore we fit all of our simulation points with the following function

$$\kappa(T; N_t) = \kappa(T_c; \text{cont}) + c_0 \cdot t + c_1 \cdot t^2 + c_2 / N_t^2 + c_3 \cdot t / N_t^2$$  \hspace{1cm} (6.2)

with fit parameters $\kappa(T_c; \text{cont}), c_0, c_1, c_2$ and $c_3$. The independent data points as well as the fitted curves (for each $N_t$ and in the continuum) are shown in Figure 5.

The $\chi^2$/d.o.f. values of the two fits are 1.19 and 1.29, respectively, indicating good fit qualities. The continuum curvatures are given by the $\kappa(T_c; \text{cont})$ fit parameter, while the relative change in the width of the transition can be read off from $-c_0$. Our final results are

$$\kappa(x_s/T^2) = 0.0089(14), \quad \kappa(\bar{\psi}\psi) = 0.0066(20)$$

$$\Delta W/W(x_s/T^2) = 0.033(16), \quad \Delta W/W(\bar{\psi}\psi) = 0.030(18)$$

The results obtained from the two quantities are consistent with each other. Using the $\kappa$ values we can give the transition lines defined by any of the observables as

$$T_c(\mu) = T_{c,\mu=0}[1 - \kappa \cdot \mu^2 / T_{c,\mu=0}^2]$$  \hspace{1cm} (6.3)

The results for $\Delta W/W$ also suggest that the transition remains a weak crossover with essentially constant strength for small to moderate chemical potentials. Actually, there is a slight increase in the width of the transition determined from both quantities. This effect is, however, very weak: the width only changes by a few percent up to $\mu \approx T_c$. This
Figure 5: The curvature $\kappa(T)$ (see definition in text) determined using the strange quark number susceptibility (left) and the renormalized chiral condensate (right), respectively. A result of the combined fit (described in the text) is shown by the gray band. The fit results for the individual $N_t = 6, 8, 10$ lattices are shown by the red, blue and green curves. The width of the gray band corresponds to the statistical uncertainty of the fit.

Our final result is shown in Figure 6. The crossover region’s extent changes little as the chemical potential increases, and within it two definitions give different curves for $T_c(\mu)$. It is useful to compare the whole picture to the freeze-out curve [34] which summarizes
experimental results on the $\{T, \mu\}$ points where hadronization of the quark-gluon plasma was observed. This curve is expected to lie in the interior of the crossover region, as is indicated by our results as well.

![Figure 6](image-url)

**Figure 6:** The crossover transition between the ‘cold’ and ‘hot’ phases is represented by the coloured area (blue and red correspond to the transition regions obtained from the chiral condensate and the strange susceptibility, respectively). The lower solid band shows the result for $T_c(\mu)$ defined through the chiral condensate and the upper one through the strange susceptibility. The width of the bands represent the statistical uncertainty of $T_c(\mu)$ for the given $\mu$ coming from the error of the curvature $\kappa$ for both observables. The dashed line is the freeze-out curve from heavy ion experiments [34]. Also indicated are with different symbols the individual measurements of the chemical freeze-out from RHIC, SPS (Super Proton Synchrotron) and AGS (Alternating Gradient Synchrotron), respectively. The center of mass energies $\sqrt{s_{NN}}$ for each are shown in the legend.

7. Acknowledgment

We thank T. Csörgő, C. Schroeder and G.I. Veres for useful discussion. Computations were performed on the BlueGene at FZ Jülich and on clusters at Wuppertal and Budapest. This work is supported in part by DFG grants SFB-TR 55, FO 502/1-2 and the EU grant (FP7/2007-2013)/ERC n°208740.
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