THE QCD PHASE DIAGRAM FOR SMALL CHEMICAL POTENTIALS

C. SCHMIDT
Fakultät für Physik, Universität Bielefeld, D-33615 Bielefeld, Germany
E-mail: schmidt@physik.uni-bielefeld.de

We compute derivatives of thermodynamic quantities with respect to \( \mu \), at \( \mu = 0 \) for 2 and 3 flavors of degenerate quark masses. This allows us to estimate the phase transition line in the \( T, \mu \) plane and quantify the influence of a non vanishing chemical potential on the equation of state by computing lines of constant energy, pressure and density. Moreover we evaluate the order of the QCD phase transition by measuring the Binder Cumulant of the chiral condensate. This gives access to the chiral critical point on the phase transition line.

1 Introduction

To understand recent heavy-ion collisions, it is mandatory to study the QCD phase diagram for high temperatures and small chemical potentials. It is well known that the order of the phase transition is strongly dependent on quark masses and chemical potential. In the space of two degenerate light quark masses \( m_{u,d} \), one heavier mass \( m_s \) and the quark chemical potential \( \mu \), one expects a critical surface, which bends over the quark mass plane and separates the regime of first order phase transitions from the crossover regime as shown in fig. 1.

To determine the order of the phase transition we compute the Binder Cumulant of the chiral condensate, \( B_4 \), at \( \mu = 0 \) for several quark masses at the pseudo-critical coupling \( \beta_c(m) \). We define \( \beta_c \) as the peak position of the chiral susceptibility. \( B_4 \) is given by

\[
B_4 = \frac{\langle (\delta \bar\psi \psi)^4 \rangle_{\beta_c,m}}{\langle (\delta \bar\psi \psi)^2 \rangle_{\beta_c,m}^2}, \quad \delta \bar\psi \psi = \bar\psi \psi - \langle \bar\psi \psi \rangle.
\]

This quantity is a renormalization group invariant quantity, with a universal value at \( m = m_{crit} \). The universality class is that of the 3d Ising model with \( B_4 = 1.604^{1,2,3} \). The critical surface is then given by the surface of constant \( B_4 = 1.604 \).

To explore the regime of \( \mu \neq 0 \) we compute derivatives of transition temperature, pressure, energy density, quark number density and Binder Cumulant with respect to \( \mu \). Direct Monte Carlo simulations for \( \mu \neq 0 \) are not possible due to the sign problem. We therefore use a reweighting method at
Figure 1. Phase boundary for the first order regime of the thermal phase transition for non-vanishing $\mu$ (left), and the line of second order phase transitions for standard staggered fermions at $\mu = 0$ (right).

$\mu = 0$ based on Taylor expansion of the fermion determinant and all observables up to order $\mu^2$. To be more precise, the expansion is given in terms of $\mu/T$ as the lattice chemical potential is given in units of the lattice cut-off, $\mu_{\text{latt}} = a\mu_{\text{phys}} \propto \mu/T$.

2 Reweighting in quark mass and chemical potential

Ferrenberg and Swendsen’s reweighting method is a very useful technique to investigate critical phenomena. Multi parameter reweighting was first applied to the problem of finite density QCD in ref. 4. We use the Taylor expanded reweighting formula up to order $\mu^2$, which is given by

$$\langle O \rangle_{(\beta,\mu)} = \frac{\langle O_0 + O_1\mu + O_2\mu^2 \exp \{R_1\mu + R_2\mu^2\} \exp \{-\Delta S_g\} \rangle}{\langle \exp \{R_1\mu + R_2\mu^2\} \exp \{-\Delta S_g\} \rangle}. \tag{2}$$

Here we have

$$R_i = \frac{N_f}{4i!} \frac{\partial^i \ln \det M(\mu)}{\partial \mu^i} \bigg|_{\mu = 0} \quad \text{and} \quad O_i = \frac{1}{i!} \frac{\partial^i O(\mu)}{\partial \mu^i} \bigg|_{\mu = 0} \tag{3}$$

We calculate the reweighting operators $R_i$ using stochastic estimators. One can easily deduce the corresponding reweighting operators for mass reweighting. We have control over the sign problem through the odd reweighting operators $R_{2j+1}$, which are purely imaginary. The phase, $\Theta$, of the fermion determinant, $\det M = |\det M| \exp \{i\Theta\}$, is in leading order given by $\Theta = \mu \text{Im}R_1$. From this we find increasing phase fluctuations for increasing volume, number of flavors, $n_f$, and for decreasing $m$ and $T$. 
In 2-flavor QCD the transition from a hadron gas to the QGP will be a continuous but rapid crossover for non vanishing quark masses and small values of $\mu$. In order to estimate the transition line we performed simulations with 2 flavors of improved fermions on a $16^3 \times 4$ lattice and quark masses of $am = 0.1$ and $am = 0.2$. From the peak positions of the Polyakov loop susceptibility and the chiral susceptibility we find $d^2 \beta_c / d\mu^2 = -1.07(24)$ and $d^2 \beta_c / d\mu^2 = -1.10(68)$ respectively, which agrees with results of ref. 7. To set the physical scale we use the string tension and obtain $a(d\beta / da) = -2.08(43)$ at $(\beta, m) = (3.65, 0.1)$. Combining these results yields

$$T_c \frac{d^2 T_c}{d\mu_q^2} = -\frac{1}{N_f^2} \frac{d^2 \beta_c}{d\mu^2} \left( \frac{d\beta}{a} \right)^{-1} = -0.14(7).$$

Derivatives of the pressure $p$ and the interaction measure $\epsilon - 3p$ are related to the quark number density $n_q$ and quark number susceptibility $\chi_s = \partial n_q / \partial \mu_q$ in the following way:

$$\frac{\partial (p/T^4)}{\partial \mu_q} = \frac{1}{VT^3} \frac{\partial \ln Z}{\partial \mu_q} = \frac{n_q}{T^4}$$

$$\frac{\partial^2 (p/T^4)}{\partial \mu_q^2} = \frac{1}{VT^3} \frac{\partial^2 \ln Z}{\partial \mu_q^2} = \frac{\chi_s}{T^4}$$

Figure 2. The transition line in 2-flavor QCD together with lines of constant energy, nuclear matter density and the freeze-out temperature (left) and a sketch of the phase diagram in 3-flavor QCD (right).
\[ \frac{\partial^2}{\partial \mu_q^2} \left( \epsilon - 3p \right) \approx \frac{1}{T^4} \frac{\partial \chi_s}{\partial \beta} \left( \frac{1}{a} \frac{\partial a}{\partial \beta} \right)^{-1}. \]  

We obtain \( T^2 \frac{\partial^2 (p/T^4)}{\partial \mu_q^2} \approx 0.69 \) and \( T^2 \frac{\partial^2 (\epsilon/T^4)}{\partial \mu_q^2} \approx 10.6 \) at \( \beta_c \) and \( am = 0.1 \). In the RHIC regime of \( \mu_q/T_c \approx 0.1 \) the deviation of \( p/T^4 \) and \( \epsilon/T^4 \) from results at \( \mu = 0 \) thus is only a 1\% effect. From the second derivatives of \( p \) and \( \epsilon \) with respect to \( \mu \) together with the derivatives with respect to \( T \), we calculate the lines of constant pressure and energy density, which are within errors parallel to the phase transition line:

\[ T \frac{dT}{d(\mu_q^2)} = \begin{cases} -0.106(21) & \text{(pressure)} \\ -0.081(20) & \text{(energy)} \end{cases}, \quad T_c \frac{dT_c}{d(\mu_q^2)} = -0.07(3). \]

The quark number density is zero at \( \mu = 0 \). For \( \mu \neq 0 \) it can be estimated via \( n_q a^3 = \mu_q a \chi_s a^2 \). This is \( n_q/T^3 = 0.693(5) \mu_q/T \) and \( n_q/T^3 = 0.490(4) \mu_q/T \) at \( am = 0.1 \) and \( am = 0.2 \), which translates into roughly 9\% and 6\% of nuclear matter density at the RHIC point. All these results are summarised in fig. 2 (left). In addition we also show the freeze-out temperature\(^{11} \). This suggest that at sufficiently large \( \mu_B \) there is the chance to observe experimentally a strongly interacting hadron gas phase, whereas for small \( \mu_B \) hadrons seem to freeze out right after the phase transition from QGP to the hadronic phase.

4 The chiral critical point

To determine the critical surface shown in fig. 1(left) we performed calculations with much lighter quark masses. For 3 flavors of improved fermions\(^6 \), a mass value of \( am = 0.005 \) and a volume of \( 12^3 \times 4 \), we measured the reweighting operators \( R_1, R_2 \) needed for reweighting in \( m \) and \( \mu \). At present we have five \( \beta \)-values, with a total number of 6100 trajectories. For \( am = 0.01 \) and \( V = 16^3 \times 4 \) we use \( R_1 = \bar{\psi} \psi \) for mass reweighting. To determine the critical mass value \( \bar{m} \), we compute \( B_4 \) as a function of \( m \). The two different volumes have an intersection point near the value of \( B_4 = 1.604 \), i.e. 3d Ising universality class. Due to the large errors we give an upper bound for the critical mass only, which is \( am < 0.0075 \), or in terms of the pion mass \( m_{PS} < 190 MeV \).

For increasing quark chemical potential \( \mu_q \) we find a decreasing Binder Cumulant. From the two partial derivatives \( \partial B_4/\partial (am) \) and \( \partial B_4/\partial (a^2 \mu^2) \), which we get from straight line fits of the reweighted data, and the assumption that \( \partial B_4/\partial (am) \) is constant in \( am \), one can compute the quantity \( \partial (am)/\partial (a^2 \mu^2) \). The first derivatives \( \partial B_4/\partial (a \mu) \) and \( \partial (am)/\partial (a \mu) \) vanish because of symmetry reasons. A jackknife analysis yields \( a^{-1} \partial m/\partial (\mu^2) = 0.82(23) \), or equivalently \( T \partial m/\partial (\mu^2) = 0.21(6) \). We thus find that the critical quark mass, \( \bar{m} \), increases.
with increasing chemical potential as anticipated in fig. 1 (left),

\[ \bar{m}(\mu) \approx m_3 + 0.21 \mu^2 / T. \]  

(9)

Here \( m_3 \) is the critical quark mass for 3 degenerate flavor at \( \mu = 0 \), which turns out to be roughly twice as large as the physical light quark masses, \( m_3 \approx 2 m_{u,d}^{\text{phys}} \). This result is shown in fig. 2 (right).

Based on these results we can give a first estimate for the location of the chiral critical point, i.e. the second order endpoint in the phase diagram shown in fig. 2 (left). To do so we use \( m_{u,d}^{\text{phys}} / T = 0.016 \), and assume that the curvature of the critical surface is the same for 3 and 2+1-flavor. In eq. 9 we should then replace \( m_3 \) by \( m_{21} \approx 4 m_{u,d}^{\text{phys}} \), which can be deduced from fig. 1 (right). We are interested in that point on the critical surface that corresponds to the physical ratio of quark masses, i.e. \( R = m_s^{\text{phys}} / m_{u,d}^{\text{phys}} = 24 \). From eq. 9 we then find \( \mu_q / T_c \approx 1.25 \), which corresponds to \( \mu_B \approx 3.75 T_c \approx 650 \) MeV and roughly coincides with the estimate given in ref. 12. Nevertheless our present uncertainties do not yet allow a reasonable error estimate on this value.

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References