The QCD phase diagram and heavy ion collisions from lattice QCD

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Abstract. The QCD phase diagram is an important ingredient to understand both the development of the early universe and the results of recent heavy ion collision experiments. At zero baryon density lattice QCD is an established tool, that provides precise theoretical results. Calculations at non zero densities however require new techniques to deal with the sign problem. In this talk I will review our recent effort to investigate QCD at non-vanishing baryon chemical potential.

1. Introduction

In current lattice QCD there are two main phase diagrams of QCD under investigation. One is at vanishing chemical potential. It shows the dependence of the order of the deconfinement transition on the quark masses resulting in the Columbia plot [1]. The second one is the $T$-$\mu_B$-plane of the phase diagram at physical quark masses, which is discussed in this proceedings. For both the inclusion of imaginary chemical potential can be helpful.

For physical quark masses and $\mu_B = 0$ the deconfinement transition has been found to be an analytical crossover [2], at a temperature of approximately 160 MeV [3, 4, 5]. The $\mu_B = 0$ axis is well investigated by lattice QCD [6]. For low chemical potential and temperature there is a hadronic phase of colour neutral bound states. At high temperatures the effective degrees of freedom are the quarks and gluons. This phase is called the quark gluon plasma. These two phases are separated by a crossover at low and zero chemical potential. The transition is expected to change to a first order transition for higher $\mu_B$ with a critical second order point in between. The position of the critical point is under investigation at the moment both by heavy ion collision experiments [7] and by theoretical calculations [8, 9]. For very large chemical potential a colour super conducting phase [10, 11] is expected.

2. Monte Carlo Simulations

To evaluate the path integral in lattice QCD Monte Carlo simulations are the usual choice. The expectation value of an observable $\mathcal{O}$ is given as

$$\langle \mathcal{O} \rangle = \frac{\int \mathcal{D}[U]|\mathcal{O} \det M e^{-S_G}}{\int \mathcal{D}[U] \det M e^{-S_G}} \quad (1)$$
Instead of using naive uniformly distributed random numbers to solve the integral (1), as that would take way to long, one rewrites the expectation value to

$$\langle O \rangle = \lim_{N \to \infty} \frac{1}{N} \sum_{n=1}^{N} O,$$

(2)

with fields that are generated according to the probability distribution

$$dP(U, \bar{\psi}\psi) = \frac{D[U] \det M e^{-S_G}}{\int D[U] \det M e^{-S_G}}.$$

(3)

This approach is called importance sampling.

The generation of configurations with this probability distribution can be achieved via different algorithms that have to meet certain requirements:

(i) The probability $T(U'|U)$ to move from $U$ to $U'$ has to be larger than zero.

(ii) The sum of all probabilities $T(U'|U)$ is normalized.

(iii) For the probability $P(U')$ for the system to be in a state $U'$ the stability equation $P(U') = \sum_{U} T(U'|U) P(U)$ is fulfilled.

(iv) For every $U$ and $U'$ it exists a $k$, so that $T^{k}(U'|U) > 0$ is fulfilled. This condition is called ergodicity.

An even stronger form of the third condition is the so called detailed balance condition: $T(U'|U) P(U) = T(U|U') P(U')$. This is fulfilled by most common algorithms.

One of the simplest algorithms that fulfills these conditions for lattice QCD is the Metropolis algorithm, that was introduced in 1953 [12]. However it is also rather inefficient and therefore hardly used in lattice simulations. For pure gauge theory, quenched QCD or any model where the action is bosonic and ultralocal the heat bath algorithm is a common choice. For SU(3) gauge theory it was introduced by N. Cabibbo and E. Marinari in 1982 [13].

The most common algorithm for full lattice QCD simulations that is also used for the generation of configurations in this contribution is the Hybrid Monte Carlo (HMC) algorithm. A detailed description of this algorithm can be found in [14]. The idea of the Hybrid Monte Carlo algorithm is to use molecular dynamics to move along hypersurfaces with constant energy in phase space by solving fictitious Hamilton equation of motion

$$\frac{dP}{dt} = -\frac{\partial H}{\partial Q}$$

$$\frac{dQ}{dt} = -\frac{\partial H}{\partial P}.$$  

(4)  

(5)

However one should note that this is not the Hamilton function of the physical system but an artificial or fictitious Hamilton function which allows for an efficient computation. To solve these equations one needs the momenta $\pi$ that are generated according to a Gaussian probability distribution. The evolution of these equations is done by Leap Frog algorithm (a description can be found in [14]) along a fictitious Monte Carlo time $\tau$. This procedure allows for large steps in phase space which reduces the autocorrelation time of the simulations. Since the calculation of the hyperplanes is done numerically the energy is not strictly conserved. Therefore the molecular dynamics needs to be combined with an accept reject step as in the Metropolis algorithm. Then the algorithm is exact for any choice of $\tau > 0$. 

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3. Chemical potential

The following arguments follow the discussion in [14]. For simulation without chemical potential there are on average the same number of particles and antiparticles. Therefore the expectation value of the overall baryon number density \( \langle n_B \rangle \) is zero. To describe a system with finite baryon density we need to introduce a finite quark chemical potential \( \mu_q \) to the Lagrangian. In the continuum this is relatively simple to achieve by adding a term of the form \( \bar{\psi} \gamma_4 \psi \). However, on the lattice, it is not that simple. Adding a similar term to the Dirac operator leads to a divergent energy density in the continuum limit [14], which is clearly unphysical. Instead one follows the idea of Hasenfratz and Karsch in [15] where the chemical potential is understood as the temporal component of an imaginary vector field. The temporal hopping term has then the form

\[
\frac{-1}{2a} \sum_{n \in \Lambda} \left( e^{\mu T} (\eta_4)_{\alpha\beta} U_4(n)_{ab} \delta_{n+4,m} + e^{-\mu T} (\eta_4)_{\alpha\beta} U_4^\dagger(n-4)_{ab} \delta_{n-4,m} \right).
\]  

(6)

It recovers the original action for \( \mu = 0 \) and at linear order in \( a\mu \) it reproduces the correct density term with \( \mu_T = a\mu N_t \). However this term breaks the \( \gamma_5 \)-hermiticity of the Dirac operator and leads for real \( \mu \) to a complex fermion determinant. Instead of the \( \gamma_5 \)-hermiticity of the Dirac operator where \( \gamma_5 D \gamma_5 = D^\dagger \) with a chemical potential one gets \( \gamma_5 D(\mu) \gamma_5 = D^\dagger(-\mu) \). This means that \( e^{-\mu_T} = f \) is replaced by \( (e^{\mu_T})^* = \frac{1}{f^*} \). For the determinant this yields

\[
\det(D(f)) = \det\left(D\left(\frac{1}{f^*}\right)\right),
\]

(7)

meaning that the determinant is only real if \( f = \frac{1}{f^*} \). For real \( f \) this is only fulfilled if \( f = e^{-\mu_T} = 1 \), and therefore \( \mu = 0 \). However if \( \mu = i\mu_I \) is chosen to be purely imaginary this yields

\[
f = e^{i\mu_I T} = \left(e^{-i\mu_I T}\right)^* = \frac{1}{f^*}.
\]

(8)

Thus the determinant is real for a purely imaginary chemical potential. As described in section 2 the fermion determinant enters in the Boltzmann weight factor which has to be real to allow a Monte Carlo simulation. There have been several ideas in lattice QCD on how to obtain results at real finite chemical potential like reweighting techniques [16, 17, 18, 19], Taylor expansion [20, 21, 22, 23, 24], density of state methods [25, 26], using the canonical ensemble [27, 28, 29], formulations with dual variables [30], Lefschetz thimbles [31, 32] or complex Langevin [33, 34]. In this work we will use the fact that while we cannot do simulations at real \( \mu \), there is no problem with introducing a purely imaginary chemical potential. From these calculations we can then do an analytical continuation form \( -\mu^2 \) to \( \mu^2 \).

4. Physical results

From the analytical continuation we gained a number of interesting physical results. The probably most obvious observable when studying the phase diagram is the temperature of the cross over. Our result for this temperature was published in [35] and is shown in fig. 1. An update for this results, even including an upper limit for the next order of the Taylor expansion of the temperature was given by the HotQCD collaboration in [36] by employing the Taylor expansion method that is relying on calculating the required derivatives at \( \mu_B = 0 \), instead of simulation at imaginary chemical potential. Another work on this topic directly comparing these two methods was done by Bonati et al. in [37].

Another important quantity is the equation of state. It is well investigated at vanishing chemical potential with good agreement between simulation with stout smeared fermions [38]
Figure 1. The extrapolation of the crossover temperature in comparison to the phenomenological modelling of experimental data for the freeze out points and a calculation by the Dyson-Schwinger equation. [35]

and HISQ fermions [39]. It also has been analysed up to temperatures of 1000 MeV, showing that the influence of the charm quark has to be taken into account when dealing with temperatures higher than \( \approx 300 \) MeV [40]. The investigation at finite chemical potential is more involved. One looking at the pressure as a Taylor expansion in \( \mu_B \):

\[
\frac{P}{T^4} = p_0 + p_2 \frac{\mu_B^2}{T^2} + p_4 \frac{\mu_B^4}{T^4} + p_6 \frac{\mu_B^6}{T^6} + \ldots
\]  

several results on the coefficients \( p_i \) have been published. The \( p_0 \) is just the pressure at vanishing chemical potential, which is well investigated as discussed above. For the next three coefficients we presented our continuum extrapolated results in [41]. The HotQCD collaboration published a continuum limit for \( p_2 \) and a continuum estimate on \( p_4 \) and \( p_6 \) in [42].

Finally the last observables discussed here are the fluctuations, defined as derivatives of the pressure with respect to various chemical potentials:

\[
\chi_{i,j,k}^{B,Q,S} = \frac{\partial^{i+j+k}(p/T^4)}{(\partial \hat{\mu}_B)^i(\partial \hat{\mu}_Q)^j(\partial \hat{\mu}_S)^k}, \quad \hat{\mu} = \frac{\mu}{T}.
\]  

Our current results on 48\(^3\)×12 lattices can be found in [43]. Results by other groups are available in [44] and [42]. These quantities are especially interesting as they can be used both to connect to experimental observables as discussed in [43] as well as to try to constrain the critical end point of the phase diagram [45, 42].

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