FLUX SIMULATION OF THE SU(3) SPIN MODEL AT FINITE CHEMICAL POTENTIAL*

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We present a Monte Carlo simulation of an effective theory for local Polyakov loops at finite temperature and density. The sign problem is overcome by mapping the partition sum to a flux representation. We determine the phase diagram of the model as a function of the temperature and the chemical potential.

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1. Introduction

Lattice QCD is a powerful tool to address non-perturbative phenomena quantitatively and, in principle, is one of the most appropriate techniques to explore the QCD phase diagram. However, at finite chemical potential, the fermion determinant becomes complex and it cannot be used as a Boltzmann weight in Monte Carlo simulations. Alternative approaches, such as reweighting, power series expansion, strong coupling/large mass expansion or analytic continuation from imaginary chemical work only for small chemical potential leaving the rest of the phase diagram unexplored. For true progress with QCD thermodynamics on the lattice, new ideas are necessary.

In this article, we explore the phase diagram of the SU(3) spin model [1], where the degrees of freedom are traced SU(3) valued spins (local Polyakov loops) as a function of temperature and chemical potential. This effective theory can be derived from full QCD using strong coupling expansion for the gluon action and hopping expansion for the fermion determinant. It is motivated by the relation of the deconfinement transition and center symmetry of pure gauge theory [2]. From the fermion determinant one takes

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into account a center symmetry breaking term which couples the chemical potential μ and gives rise to a sign problem at finite μ . However, in this model, the sign problem can be solved by exactly rewriting the partition sum in terms of flux variables [4, 5].

2. Center effective theory

The action of the center effective theory has the form

$$S = -\sum_{x} \left(\tau \sum_{\nu=1}^{3} [P(x)P(x+\hat{\nu})^{*} + \text{c.c.}] + \kappa \left[e^{\mu}P(x) + e^{-\mu}P(x)^{*} \right] \right). \quad (1)$$

The degrees of freedom P(x) are the traced SU(3) variables $P(x) = \operatorname{Tr} L(x)$ with $L(x) \in \operatorname{SU}(3)$ attached to the sites x of a three-dimensional cubic lattice with periodic boundary conditions. By $\hat{\nu}$ we denote the unit vector in ν -direction, with $\nu = 1, 2, 3$. The first term of the action, i.e., the nearest neighbor interaction term, can be obtained as the leading contribution in the strong coupling expansion of the gauge action. This term is invariant under center transformations $P(x) \to zP(x)$ with $z \in \mathbb{Z}_3$. The parameter τ depends on temperature (it increases with T) and is real and positive. The second term, referred to as the magnetic term, is obtained as the leading contribution in the hopping expansion (large mass expansion) of the fermion determinant. The real and positive parameter κ is proportional to the number of flavors and depends on the fermion mass (it decreases with m_q). The magnetic term breaks center symmetry explicitly and is complex when the chemical potential μ is non-zero, thus generating a sign problem.

The grand canonical partition function of the model described by (1) is obtained by integrating the Boltzmann factor $e^{-S[L]}$ over all configurations of the Polyakov loop variables. The corresponding measure is a product over the reduced Haar measures dL(x) at the sites x. Thus

$$Z = \prod_{x} \int_{SU(3)} dL(x) e^{-S[L]} = \int D[L] e^{-S[L]}.$$
 (2)

Equations (1) and (2) define the SU(3) effective theory.

3. Solving the sign problem

To overcome the sign problem we apply high temperature expansion techniques and map the theory onto a flux representation, where the partition function is rewritten in terms of new degrees of freedom, so-called flux variables. Here, we outline the general strategy for the derivation of the flux representation (for the details see [5]). The general steps are:

- 1. Write the Boltzmann weight in a factorized form and expand the exponentials for individual links and sites.
 - Nearest neighbor term (links):

$$e^{\tau P(x)P(x+\hat{\nu})^{\star}} \to \sum_{l_{x,\nu}} \frac{\tau^{l_{x,\nu}}}{l_{x,\nu}!} \left[P(x)P(x+\hat{\nu})^{\star} \right]^{l_{x,\nu}} ,$$

$$e^{\tau P(x)^{\star}P(x+\hat{\nu})} \to \sum_{\bar{l}_{x,\nu}} \frac{\tau^{\bar{l}_{x,\nu}}}{\bar{l}_{x,\nu}!} \left[P(x)^{\star}P(x+\hat{\nu}) \right]^{\bar{l}_{x,\nu}} .$$

• Magnetic term (sites), we use $\eta \equiv \kappa e^{\mu}$ and $\bar{\eta} \equiv \kappa e^{-\mu}$:

$$e^{\eta P(x)} \rightarrow \sum_{s_x} \frac{\eta^{s_x}}{s_x!} P(x)^{s_x}, \qquad e^{\overline{\eta} P(x)^{\star}} \rightarrow \sum_{\overline{s}_x} \frac{\overline{\eta}^{\overline{s}_x}}{\overline{s}_x!} P(x)^{\star \overline{s}_x}.$$

2. Rewrite the partition function as:

$$Z = \sum_{\{l,\bar{l}\}} \sum_{\{s,\bar{s}\}} \left(\prod_{\overline{x},\nu} \frac{\tau^{l_{x,\nu} + \overline{l}_{x,\nu}}}{l_{x,\nu}! \overline{l}_{x,\nu}!} \right) \left(\prod_{x} \frac{\eta^{s_x} \overline{\eta}^{\overline{s}_x}}{s_x! \overline{s}_x!} \int dP(x) P(x)^{f(x)} P(x)^{\star \overline{f}(x)} \right),$$
where $f(x) = \sum_{\nu=1}^{3} [l_{x,\nu} + \overline{l}_{x-\hat{\nu},\nu}] + s_x$ and $\overline{f}(x) = \sum_{\nu=1}^{3} [l_{x-\hat{\nu},\nu} + \overline{l}_{x,\nu}] + \overline{s}_x$ denote two types of fluxes at a site x of the lattice.

- 3. After integrating out the SU(3) variables L(x) [3], the new form of the partition sum depends only on the flux variables:
 - Dimers $l_{x,\nu}, \bar{l}_{x,\nu} \in [0, +\infty[$, living on the links (x, ν) .
 - Monomers $s_x, \overline{s}_x \in [0, +\infty[$, living on the sites x.
- 4. The flux variables $l_{x,\nu}, \bar{l}_{x,\nu}, s_x, \bar{s}_x$ are the new degrees of freedom and $\sum_{\{l,\bar{l}\}} \sum_{\{s,\bar{s}\}}$ denotes the sum over all their configurations. The flux variables are subject to a constraint which forces the total flux $f(x) \bar{f}(x)$ to be a multiple of 3 at each site x.

4. Numerical analysis

For the analysis, we performed simulations with a local Monte Carlo update on 10^3 , 16^3 and 20^3 lattices and focused on the bulk observables internal energy U and the magnetization P (which is identified with the Polyakov loop of QCD), as well as their fluctuations C (heat capacity) and χ_P (Polyakov loop susceptibility).

First, we performed several checks of the flux representation and the algorithm. Fig. 1 shows that for small μ and τ the data obtained from the simulation (circles) nicely approaches the analytical results from a perturbative expansion in τ (lines). We plot P and χ_P for $\tau=0.001$ and three different values of κ as a function of the chemical potential. The same comparison is shown in Fig. 3 (left), where the solid curves at the bottom are the positions of the maxima from the perturbative expansion.

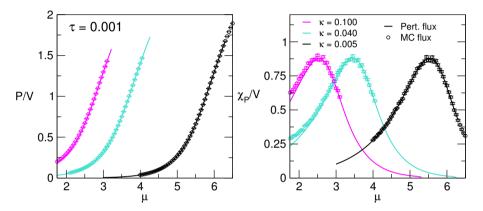


Fig. 1. P (left) and χ_P (right) for $\kappa = 0.1, 0.04$ and 0.005 and $\tau = 0.001$. We compare the results from the Monte Carlo simulation on a 10^3 lattice (circles) and perturbative expansion in τ (lines).

We also compared our results to other approaches. Fig. 2 shows that the flux results and the data from a complex Langevin calculation [6] agree very well, and for $\mu = 0$ also with the results from a conventional simulation in the spin representation. The discrepancy at $\tau = 0.132$ is solved when a higher-order algorithm is used for the two values, $\mu^2 = 0.0$ and 0.2 (crosses).

To explore the phase boundaries in the τ - μ plane, we identified the positions of the maxima of $\chi_{\rm P}$ and C. Subsequently, we used two methods to determine the nature of the transitions: first we studied the histograms of U and P to search for a double peak behavior characteristic of a first order transition, and secondly we analyzed the volume scaling of C and $\chi_{\rm P}$. Fig. 3 (left) shows the positions of the maxima of $\chi_{\rm P}$ in the τ - μ plane for $\kappa=0.1,\ 0.04,\ 0.02$ and 0.005. We find that there is a first order phase transition for small μ and $\kappa<\kappa_{\rm c}$ (triangles), while the rest of the transition lines shows a crossover behavior (circles). Our estimate for the critical point for $\mu=0$ is $(\tau_{\rm c},\kappa_{\rm c})=(0.1331(1),0.016(2))$. This value is different from a mean field analysis of the SU(3) spin model [7], where the critical point was reported to be at $\kappa=0.059$. However, in [8] it was shown that when considering higher order corrections the value $\kappa_{\rm c}$ from the mean field approach

decreases. Fig. 3 (right) shows the positions of the maxima of $\chi_{\rm P}$ and C, demonstrating that the crossover region (manifest also in different positions for the maxima of $\chi_{\rm P}$ and C) becomes wider with increasing μ .

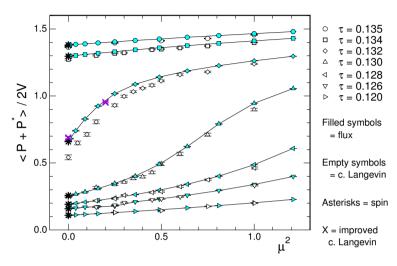


Fig. 2. Comparison of $\langle P+P^*\rangle/2V$ from the flux simulation (filled symbols) to the results from the complex Langevin approach (empty symbols and two high accuracy data points are marked with crosses). For $\mu=0$ we also added the results from a simulation in the conventional spin approach (asterisks). We compare data at different values of τ as a function of μ^2 for $\kappa=0.02$ on lattices of size 10^3 .

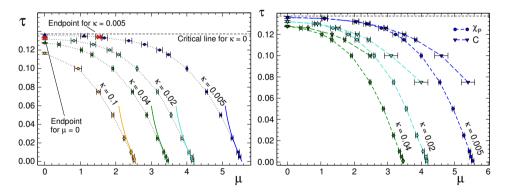


Fig. 3. Left: Phase diagram obtained from the maxima of $\chi_{\rm P}$ for 4 values of κ . The horizontal line marks the critical τ for $\kappa=0$, and the curves below it are the results from a τ expansion. The point (red) for $\kappa=0$ is the critical endpoint. Right: Comparison of the phase boundaries obtained from the maxima of $\chi_{\rm P}$ and C for three values of κ .

5. Conclusions

We have studied an effective theory for the Polyakov loop at finite temperature and density. Mapping the theory onto a flux representation enables us to have a model free of the sign problem and opens the possibility to use Monte Carlo techniques. For large values of κ (physical case) the transition is of a smooth crossover type and we conclude that center symmetry alone does not provide a mechanism for first order behavior in the QCD phase diagram.

We also compared the recently published results from a complex Langevin simulation of the SU(3) spin model [6] to the data from our flux simulation. We find very good agreement between the two methods which is a valuable test for both, the flux and the complex Langevin approach.

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