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THE QCD PHASE DIAGRAM FROM THE LATTICE*

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We present a phase diagram of effective Polyakov line actions, derived from the SU(3) lattice gauge theory with 695 MeV dynamical staggered quarks. We find a phase-transition line in the temperature–density plane. The derivation is via the method of relative weights and the effective theories are solved at finite chemical potential by mean-field theory.

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1. Introduction

One of the most active areas in strong-interaction physics concerns the behavior of QCD in extreme conditions, *i.e.* high temperature and/or high baryon density. At high temperatures, we enter the realm of the quark–gluon plasma, whose properties have been or will be probed by experiments at RHIC, the LHC, and the FAIR facility (now under construction). Not much is known for sure about hadronic matter at high baryon density. QCD is believed to have a complex phase structure in the temperature-density plane, and a number of exotic phases (quarkyonic, glasma, color–flavor locked superconductor *etc.*) have been suggested. One would especially like to know the position of the critical endpoint of the confinement–deconfinement transition. Many talks on the subject of QCD in extreme environments begin

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with a sketch of the possible phase diagram, but such sketches are, so far, all conjecture. Nobody knows whether these exotic phases really exist, or exactly where they are located in the temperature/density plane. So the first order of business, for a theorist, is to nail down the phase diagram.

By far, the most important tool in the investigation of non-perturbative QCD is the method of importance sampling in lattice Monte Carlo simulations. However, when one attempts to apply this tool to study QCD at high baryon density, a serious obstacle — the "sign problem" — is encountered. Different strategies were explored, and the reviews at the yearly lattice conferences [1–10] summarize the progress. Finite densities are introduced in statistical systems via the introduction of a chemical potential, but when this standard method is applied in QCD, the fermion determinant becomes complex and cannot be interpreted as a probability measure. Then standard importance sampling, *e.g.* via the hybrid Monte Carlo method, breaks down completely, and some other method or methods must be devised to handle the problem of complex actions.

Our approach to the sign problem in QCD is to map QCD with a chemical potential into a simpler effective theory, namely, the effective Polyakov line action (henceforth "PLA"), via the relative weights method and then deal with the sign problem via mean-field theory, which is a surprisingly accurate method for solving effective actions of this kind [11]. The phase diagram of the effective theory will mirror the phase diagram of the underlying gauge theory. The method was successfully tested in SU(2) and SU(3) pure gauge and gauge-Higgs theories [12–14], and first results with dynamical fermions were presented in [15–19].

2. Formalism and methodology

The effective Polyakov line action S_P is the theory obtained by integrating out all degrees of freedom of the lattice gauge theory, under the constraint that the Polyakov line holonomies are held fixed. It is convenient to implement this constraint in temporal gauge ($U_0(\boldsymbol{x}, t \neq 0) = \mathbb{1}$), so that

$$\exp\left[S_\mathrm{P}\left[U_{\vec{x}}, U^\dagger_{\vec{x}}\right]\right] = \int DU_0(\vec{x},0) DU_k D\phi \left\{\prod_{\vec{x}} \delta\left[U_{\vec{x}} - U_0(\vec{x},0)\right]\right\} e^{S_\mathrm{L}} \,, \quad (1)$$

where ϕ denotes any matter fields, scalar or fermionic, coupled to the gauge field, and S_L is the SU(3) lattice action. To all orders in a strong-coupling/hopping parameter expansion, the relationship between the PLA at zero chemical potential $\mu = 0$, and the PLA corresponding to a lattice gauge theory at finite chemical potential, is given by

$$S^\mu_\mathrm{P}\left[U_{\vec{x}}, U^\dagger_{\vec{x}}\right] = S^{\mu=0}_\mathrm{P}\left[e^{N_t\mu} U_{\vec{x}}, e^{-N_t\mu} U^\dagger_{\vec{x}}\right] . \quad (2)$$

So the immediate problem is to determine the PLA at $\mu = 0$. Let us define the Polyakov line in an SU(N) theory to refer to the trace of the Polyakov line holonomy $P_{\vec{x}} \equiv \frac{1}{N}\mathrm{Tr}[U_{\vec{x}}]$. Relative weights enable us to compute the derivative of the effective action S_P along any path

$$\left(\frac{\mathrm{d}S_\mathrm{P}}{\mathrm{d}\lambda}\right)_{\lambda=\lambda_0} \approx \frac{\Delta S_\mathrm{P}}{\Delta\lambda} \tag{3}$$

at any point $\{U_{\vec{x}}(\lambda_0)\}$ in the configuration space of all $U_{\vec{x}}$ on the lattice volume, parametrized by λ. We compute the derivatives of the effective action, by the relative weights method, with respect to the Fourier ("momentum") components $a_{\vec{k}}$ of the Polyakov line configurations $P_{\vec{x}} = \sum_{\vec{k}} a_{\vec{k}} e^{i\vec{k}\cdot\vec{x}}$. The procedure is to run a standard Monte Carlo simulation, generate a configuration of Polyakov line holonomies $U_{\vec{x}}$, and compute the Polyakov lines $P_{\vec{x}}$. We then set the momentum mode $a_{\vec{k}} = 0$ in this configuration to zero, resulting in the modified configuration $\widetilde{P}_{\vec{x}} = P_{\vec{x}} - \left(\frac{1}{L^3}\sum_{\vec{y}} P_{\vec{y}} e^{-i\vec{k}\cdot\vec{y}}\right) e^{i\vec{k}\cdot\vec{x}}$, and define

$$P''_{\vec{x}} = \left(\alpha - \frac{1}{2}\Delta\alpha\right) e^{i\vec{k}\cdot\vec{x}} + f\widetilde{P}_x\,, \qquad P'_{\vec{x}} = \left(\alpha + \frac{1}{2}\Delta\alpha\right) e^{i\vec{k}\cdot\vec{x}} + f\widetilde{P}_x\,, \tag{4}$$

where f is a constant close to one ($f = 1$ is only possible in the large volume, $\alpha \to 0$ limit). From the holonomy configurations U''_x, U'_x, we compute derivatives of S_P with respect to the real part $a^\mathrm{R}_{\vec{k}}$ of the Fourier components $a_{\vec{k}}$ by defining $\Delta S_\mathrm{P} = S_\mathrm{P}[U'_{\vec{x}}] - S_\mathrm{P}[U''_{\vec{x}}]$, hence we have from (1)

$$e^{\Delta S_\mathrm{P}} = \frac{\int DU_k D\phi e^{S'_\mathrm{L}}}{\int DU_k D\phi e^{S''_\mathrm{L}}} = \frac{\int DU_k D\phi \exp\left[S'_\mathrm{L} - S''_\mathrm{L}\right] e^{S''_\mathrm{L}}}{\int DU_k D\phi e^{S''_\mathrm{L}}} = \left\langle \exp\left[S'_\mathrm{L} - S''_\mathrm{L}\right]\right\rangle''\,. \tag{5}$$

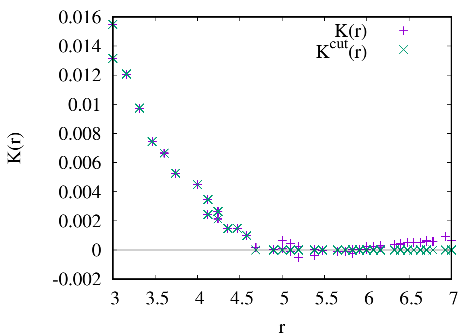
The expectation value is straightforward to compute numerically, by fixing the Polyakov holonomies and calculating the action differences, and from the logarithm, we determine ΔS_P. Our proposal is to fit the relative weights data to an Ansatz for S_P based on the massive quark effective action [20]

$$\begin{aligned} S_\mathrm{P}[U_{\vec{x}}] \;=\; & \sum_{\vec{x},\vec{y}} P_{\vec{x}} K(\vec{x}-\vec{y}) P_{\vec{y}} \\ & + p\sum_{\vec{x}} \Big\{ \log\left(1 + h e^{\mu/T}\mathrm{Tr}[U_{\vec{x}}] + h^2 e^{2\mu/T}\mathrm{Tr}\left[U^\dagger_{\vec{x}}\right] + h^3 e^{3\mu/T}\right) \\ & + \log\left(1 + h e^{-\mu/T}\mathrm{Tr}[U_{\vec{x}}] + h^2 e^{-2\mu/T}\mathrm{Tr}\left[U^\dagger_{\vec{x}}\right] + h^3 e^{-3\mu/T}\right)\Big\}\,, \end{aligned} \tag{6}$$

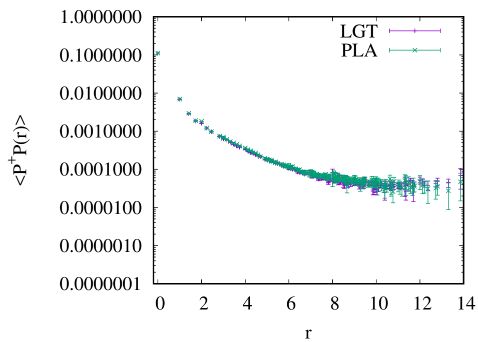
where both the kernel $K(\vec{x}-\vec{y})$ and the parameter h are to be determined by the relative weights method. The full action is surely more complicated than this Ansatz; the assumption is that these terms in the action are dominant, and the effect of a lighter quark mass is mainly absorbed into the parameter h and kernel $K(\vec{x}-\vec{y})$. We then have the derivative of the action with respect to momentum modes $a_{\vec{k}}$ of the Polyakov lines

$$\frac{1}{L^3}\left(\frac{\partial S_{\mathrm{P}}}{\partial a^{\mathrm{R}}_{\vec{k}}}\right)_{a_{\vec{k}}=\alpha} = 2\widetilde{K}\left(\vec{k}\right)\alpha + \frac{p}{L^3}\sum_{\vec{x}}\left(3he^{i\vec{k}\cdot\vec{x}} + 3h^2 e^{-i\vec{k}\cdot\vec{x}} + \mathrm{c.c.}\right) . \quad (7)$$

The left-hand side is computed via relative weights at a variety of $\alpha = 0.01, \ldots, 0.06$, and plotting those results *vs.* α, $K(\vec{k})$ is determined from the slope, while h is given by the intercept at $\alpha = 0$ from the zero mode $k = 0$, since the second term vanishes for $k \neq 0$. From the kernel $K(\vec{k})$ in the momentum space, we derive the kernel $K(\vec{x}-\vec{y})$ via inverse Fourier transformation and find that it basically vanishes above $r \approx 4.6$, see figure 1 (a), hence we introduce a cutoff R_{cut} and set the kernel to zero for $r > R_{\mathrm{cut}} = 4.6$.



(a)

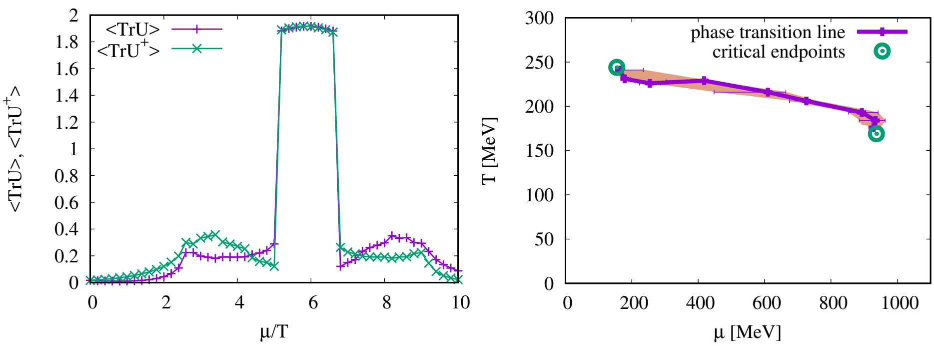


(b)

Fig. 1. (a) The kernel $K(r) = K(\vec{x}-\vec{y})$ of the PLA for various lattice sizes and an infinite volume fit. (b) Polyakov line correlators from the lattice and PLA simulations.

3. Results from mean-field theory

We derive effective Polyakov line actions from lattice simulations of Wilson gauge action and dynamical staggered fermions, for a variety of temperatures and lattice masses corresponding to a physical quark mass $m_q = 695$ MeV. A first consistency check of our PLA simulations is that we reproduce the correct Polyakov line correlator of the underlying lattice gauge theory, as shown in figure 1 (b) for $\beta = 5.7$. For $\mu \neq 0$, the effective PLA has still a sign problem, which we solve via mean-field theory as discussed in [21, 22]. The treatment of SU(3) spin models at finite μ is just a minor variation of the standard mean-field theory at zero chemical potential. The basic idea that each spin is effectively coupled to the average spin on the lattice, not just nearest neighbors, is favored by the effective PLA with the non-local kernel $K(\vec{x}-\vec{y})$. We introduce two magnetizations for $\mathrm{Tr}(U)$ and $\mathrm{Tr}(U^\dagger)$ which are determined by minimizing the free energy. A check of the mean-field approach is that we reproduce the correct expectation value of the Polyakov loop from LGT at for $\mu = 0$. An example for the mean-field results of the PLA from LGT at $\beta = 5.7$ is shown in figure 2 (a), showing a phase transition at $\mu/T \approx 5$. The transition points are plotted in figure 2 (b), yielding a first phase diagram for dynamical quarks.



(a) (b)

Fig. 2. (a) Polyakov lines from mean-field analysis of the PLA derived from LGT at $\beta = 5.7$ Wilson gauge coupling and dynamical staggered fermions. (b) Preliminary phase diagram for $m_q = 695$ MeV, showing a phase transition line ending in two endpoints. We cannot rule out that a transition line reappears at lower temperatures, or that the second endpoint is absent for light quarks.

4. Conclusions

We have found a first-order phase transition line for SU(3) gauge theory with dynamical unrooted staggered fermions of mass 695 MeV in the plane of chemical potential μ and temperature T, which agrees very well with results from analytic continuation of imaginary μ [23].

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