THE PHASE DIAGRAM OF HEAVY DENSE QCD WITH COMPLEX LANGEVIN SIMULATIONS*

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The sign problem of QCD prevents standard lattice simulations to determine the phase diagram of strong interactions with a finite chemical potential directly. Complex Langevin simulations provide an alternative method to sample path integrals with complex weights. We report on our ongoing project to determine the phase diagram of QCD in the limit of heavy quarks (HDQCD) using Complex Langevin simulations.

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1. Introduction

The phase diagram of strong interactions is, despite various efforts, still largely unknown. Several states of matter are expected to be present, which are relevant to many phenomena such as the quark–gluon plasma, neutron stars and the evolution of the universe after the Big Bang. A possible scenario of the QCD phase diagram is sketched in Fig. 1. A theoretical pre-

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Fig. 1. A scenario of the QCD phase diagram.

diction can guide heavy-ion collision experiments, which might lead to the discovery of different states of matter. However, the *sign problem* leads to a path integral with a complex weight and thereby prevents direct determination using standard lattice simulation based on importance sampling. Complex Langevin simulations, based on stochastic quantisation, might provide a viable solution to sample path integrals with complex weights [1–16]. In the following, we will present an update on our project to determine the phase diagram of heavy dense QCD (HDQCD), an approximation of QCD in the limit of heavy quarks, from first principles.

2. Complex Langevin simulation

Here, we summarise the basics of the Complex Langevin method, more details can be found in [4–7]. In analogy to the Hybrid Monte Carlo method, we introduce the so-called Langevin time t, which labels the evolution of observables and degrees of freedom in this stochastic quantisation. Integrating out the fermion fields leads to a path integral with a complex weight

$$Z = \int DU |\det D| e^{i\Theta} e^{-S_{\rm YM}(U)}, \qquad (1)$$

if the chemical potential is real and non-zero, since

$$[\det D(\mu)]^* = \det D(-\mu^*).$$
 (2)

To incorporate the complex nature of the path integral in our simulations, we extend the gauge group from SU(3) to SL(3, \mathbb{C}). For small step-sizes ϵ , the gauge links $U_{\mu x}$ are evolved by

$$U_{\mu x}(t+\epsilon) = R(t) U_{\mu x}(t), \qquad (3)$$

where the update matrix R(t) can be written in term of the Gell-Mann matrices λ and stochastic Gaussian white noise η

$$R(t) = \exp\left[i\lambda\left(-\epsilon D_U S + \sqrt{\epsilon} \eta\right)\right],\tag{4}$$

where the action includes the logarithm of the determinant. Here, we study QCD in the limit of heavy quarks, for which the fermion determinant can be written in terms of the (conjugate) Polyakov loops $\mathcal{P}_{\vec{x}}$ and $\mathcal{P}_{\vec{\tau}}^{-1}$

$$\det D(\mu) = \prod_{\vec{x}} \det \left(1 + h \, e^{\mu/T} \, \mathcal{P}_{\vec{x}} \right)^2 \det \left(1 + h \, e^{-\mu/T} \, \mathcal{P}_{\vec{x}}^{-1} \right)^2 \,, \qquad (5)$$

with $h = (2 \kappa)^{N_{\tau}}$. For the gluonic part of the action, we use the full Wilson gauge action. To avoid runaway trajectories into the non-compact extension of SU(3), we apply adaptive step-size scaling [5] and adaptive gauge cooling [6,7]. Too many large excursions into the imaginary directions have been identified to cause the Complex Langevin method to fail by converging to incorrect results. It can be shown that if the action is holomorphic and suitably confined in the complex of extension of SU(3), Complex Langevin simulations are expected to converge to the correct results [9,10]. The logarithm of the determinant causes poles in the derivative of the action, and thereby prevents the aforementioned proof to be applied. Nevertheless, recent work [11–13] has shown that especially for large quark masses this ambiguity will not affect Complex Langevin dynamics. We still monitor the distributions of the observables and the so-called unitnorm,

unitnorm = Tr
$$\left(UU^{\dagger} - \mathbb{I}\right)^2$$
, (6)

to avoid runaway trajectories in our simulations.

3. Numerical setup and results

We study the phase diagram of heavy dense QCD for fixed lattice spacing and the simulation parameters are given in Table I. For HDQCD, the

TABLE I

Summary of simulation parameters.

expected critical chemical potential μ_c (in lattice units) is related to the bare quark mass by

$$\mu_{\rm c} \sim m_q \equiv -\ln(2\kappa) = 2.53\,.\tag{7}$$

We have improved our previous results [14] by considering larger Langevin trajectories, with a maximum Langevin time of 500. The interval up to 100 Langevin time has been discarded to remove thermalisation effects. Using adaptive step-sizes ϵ , we find typical values of $\epsilon \sim 10^{-4}$. We have determined the observables every $\delta t = 10^{-2}$, which corresponds to approximately 100 sweeps in between measurements. Including auto-correlation, we have at least 2000 independent configurations for each simulation. Figure 2 shows



Fig. 2. The Polyakov loop as function of T and μ .

the expectation value of the Polyakov loop as a function of temperature Tand the chemical potential μ . The temperature has been converted to physical units using the lattice spacing of $a \sim 0.15$ fm, which has been determined using the Wilson flow [15, 17]. Each black point in Fig. 2 is the result of a dedicated simulation. The Polyakov loop shows a clear signal for the deconfinement transition and a transition to higher densities. At high densities, $\mu/m_q \geq 1$, the Polyakov loop drops again. This behaviour is an expected lattice artefact, at which every lattice site has been filled with the maximum number of fermions allowed by the Pauli principle. The coloured surface is a cubic interpolation to the individual simulations. The resolution in temperature is quite limited in the fixed lattice spacing approach, since the temporal extend is by construction an integer. Figure 3 shows the equivalent plot for the susceptibility of the Polyakov loop, which directly maps out the boundary of the phase diagram of HDQCD. The deconfinement transition appears to be quite broad, which is caused by our limited resolution for large



Fig. 3. The Polyakov loop susceptibility as function of T and μ .

temperatures and the subsequent interpolation. We find a clearer signal for the transition to higher densities, which almost disappears on the plotted scale, using the susceptibility of the fermion density

$$n = \frac{1}{N_{\tau} N_s^3} \frac{\partial \ln Z}{\partial \mu} \,. \tag{8}$$

4. Conclusions and outlook

Complex Langevin simulations provide a viable method to determine the phase diagram of heavy dense QCD from first principles. Further work includes the identification of the order of the transitions by varying the simulation spatial volume and studying the Binder cumulant. Simulation at different lattice spacing will improve the resolution in the temporal direction and allow to asses the size of lattice artefacts. The ultimate goal is to repeat these simulation for fully dynamical QCD [15,16] and study the phase diagram of QCD itself. In perspective of this goal, the work here can be considered as blueprint for further studies and as proof of principle. We are grateful for the computing resources made available by HPC Wales and by STFC through DiRAC computing facilities. This work is supported by STFC, the Royal Society, the Wolfson Foundation and the Leverhulme Trust. F.A. is grateful for the support through the Brazilian government program "Science without Borders" under scholarship number Bex 9463/13-5. B.J. acknowledges financial support from the College of Science Research Fund at Swansea University.

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