Progress in complex Langevin simulations of full QCD at nonzero density

Dénes Sexty

Institut für Theoretische Physik, Universität Heidelberg, Heidelberg, Germany

Abstract

Progress in the application of the complex Langevin method to full QCD at non-zero chemical potential is reported. The method evades the sign problem which makes naive simulations at nonzero density impossible. The procedure 'gauge cooling' is used to stabilize the simulations at small enough lattice spacings. The method allows simulations also at high densities, all the way up to saturation. Simulations in a systematic hopping parameter expansion are also performed and good convergence is observed, validating the full as well as the expanded simulations.

Keywords: Lattice QCD, Finite chemical potential, Complex Langevin

1. Introduction

In recent years, we have seen the great success of lattice QCD, a first-principles non-perturbative approach with well controlled approximations. However, the naive application of this method requires that we formulate the theory using a path integral with a positive definite measure,

\[ Z(\mu) = \int DU e^{-S_g[U]} \det M(\mu, U)^{N_F}, \quad (1) \]

where \( S_g[U] \) is the gauge action and \( M(\mu, U) \) is the fermion matrix which describes \( N_F \) quark degrees of freedom. For nonzero chemical potential \( \mu > 0 \), the fermionic determinant is non positive definite, therefore importance sampling methods are not applicable. This is known as the 'sign problem'. Various methods have been invented to negate the sign problem, such as reweighting, Taylor expansion, analytical continuation from imaginary chemical potential, etc. but these are mostly successful in the low chemical potential region, \( \mu/T \ll 1 \) (for a review, see [1, 2]).

Recent progress in complex Langevin (CL) dynamics has shown [3, 4] that one can evade the QCD sign problem by the complexification of the variables. This method allows direct simulations of a theory with complex action without any sign or overlap problem (see e.g. applications to Bose gas [5], Yang-Mills theory with \( \Theta \)-term [6], real-time physics [7]). The complex Langevin simulations are based on on setting up a stochastic process on the complexification of the original field manifold [8, 9]. The averages of the original theory are recovered using the principle of analytic continuation. In some cases, the process is known to produce wrong results. The understanding of this behavior has progressed in the recent years: one can formally prove the correctness of the approach [10], provided a few conditions are met, such as the holomorphicity of the action and the fast falloff of the distribution of the variables in the complexified configuration space. In the case of QCD, the action we simulate \( S_{\text{eff}}[U] = S_g[U] + \ln \det M(\mu, U) \) is non-holomorphic, it has a branch cut. This leads to a meromorphic drift term. Poles in the drift may lead to wrong
convergence of the process, as shown in nontrivial, soluble models [11]. Recent evidence suggests that in the case of QCD, at least in some region of the parameters, this non-analiticity does not lead to problems, as seen by comparing two versions of the theory, the full and the expanded in which there are no singularities (see below and in [12]).

An essential ingredient of the complex Langevin simulations of gauge theories is gauge cooling [3, 13]. The complexification of the field manifold from SU(3) to SL(3,C) gives rise to problems in the naive application of the complex Langevin equation, as the link variables try to explore the complexified, non-compact manifold SL(3,C). This undesirable behavior can be countered by using the gauge freedom in the complexified manifold to move the configuration closer to the original SU(3) manifold. This is achieved by decreasing the ‘unitarity norm’ \( \sum_{x,\nu} \text{Tr}(U_{x,\nu}U^+_{x,\nu}) \) using gauge transformations, i.e. searching for the minimum of the unitarity norm by changing the configuration in the direction of the steepest descent. The dynamical updates are interspersed with gauge cooling steps which keep the complexified dynamics stable.

One observes that gauge cooling succeeds in controlling the process in the complexified field manifold such that a stable behavior is seen, without dangerous ‘skirts’ in the distribution of the variables, if the \( \beta \) parameter of the action is not too small. The limiting value seems to depend very mildly on the lattice size [14], so in practice this limitation means that there is an upper limit on the allowed lattice spacings that one can use. This value is around \( a_{\text{max}} = 0.1 - 0.2 \) fm, depending on the fermion content of the theory. Lower temperatures are thus more expensive to simulate, as they require larger lattices.

Besides full QCD, we also study an approximation to QCD called HDQCD in which the spatial hopping parameter \( \kappa_s \) is set to zero. This is formally justified in the double limit \( \kappa \to 0, \mu \to \infty \), with \( \zeta = 2\kappa e^{\mu} \) fixed [15]. HDQCD represents the leading order (LO) in a systematic expansion of the fermionic determinant. This has been extended to next-to-leading order (NLO) using the loop expansion [15, 16], and also to higher orders in combination with the strong coupling expansion [17]. However, going to higher orders is difficult, as one has to consider possible fermionic loops and their combinatorial factors. We recently presented an expansion which allows systematic calculation of fermionic corrections to all orders [12], using the full gauge action with CL dynamics to negate the remaining sign problem at nonzero chemical potential. This approach shows explicitly the convergence of the expansion, therefore it validates also the full theory where theoretical understanding of the meromorphic drift is still lacking.

---

Figure 1. The fermionic density ((1/\( N^3 N_t \))\( \partial \ln Z/\partial \mu \)), in units of the saturation density), the Polyakov loops, and the chiral condensate \( \langle \bar{\psi} \psi \rangle \) (shifted by an arbitrary value for better visibility) in full QCD using 1 flavor of Wilson fermion at fixed temperature as a function of the chemical potential.
2. Results

The method has been implemented for staggered fermions in [4]. Here results using unimproved Wilson fermions are presented, using the fermion matrix

\[ M(x, y) = 1 - \sum_{\nu=1}^{4} \kappa_\nu \left( (1 - \gamma_\nu) \exp(\delta_\nu \mu) U_\nu(x) \delta_{y,x+a_\nu} + (1 + \gamma_\nu) \exp(-\delta_\nu \mu) U_{-\nu}(y) \delta_{y,x-a_\nu} \right), \]  

(2)

with the hopping parameters \( \kappa_\nu \) (the spatial hopping \( \kappa_1 = \kappa_2 = \kappa_3 \)) and Euclidean Gamma-matrices \( \gamma_\nu \). The contribution of the fermions to the drift term is calculated using a noisy estimator similarly to the staggered case, where the numerical cost is one conjugate gradient solution per update.

The response of the lattice system to the chemical potential is demonstrated on Fig. 1. The fermionic density rises to a large value, until all the available states on the lattice are filled, and the system is saturated. The Polyakov loops signal deconfinement, but decay again when lattice effects of the saturation become important, their peaks being close to the point of half filling, when every other fermionic state is filled on the average.

On Fig. 2 we compare the HDQCD approximation to the full QCD using one flavor of Wilson fermion. One observes that the qualitative behavior is very similar, both theories exhibit the phenomenon of saturation.

We define the \( \kappa \)-expansion by rewriting the fermionic determinant

\[ \det M = \det(1 - \kappa Q) = \exp \sum_{n=1}^{\infty} \frac{\kappa^n}{n} \text{Tr} Q^n, \]  

(3)

where \( Q \) is the hopping part of the matrix, and the \( \kappa_* \)-expansion by first pulling out the temporal hopping terms \( R \)

\[ \det M = \det(1 - R - \kappa_* S) = \det(1 - R) \left( 1 - \frac{\kappa_* S}{1 - R} \right) = \det(1 - R) \exp \sum_{n=1}^{\infty} \frac{\kappa_n^n}{n} \text{Tr} \left( \frac{\kappa_*}{1 - R} S \right)^n, \]  

(4)

leaving an expansion in terms of the spatial hopping matrix \( S \). These expansions can be conveniently implemented in the complex Langevin dynamics using noisy estimators [12]. On Fig. 3 the performance of these expansions is demonstrated. The \( \kappa \)-expansion is slightly cheaper to calculate, but converges only at small chemical potentials, as the expansion includes terms which are proportional to \( e^\mu \). In contrast, in the \( \kappa_* \)-expansion the \( \mu \) dependent terms are pulled out to be dealt with analytically, so it has better convergence properties at large \( \mu \), but it is more expensive, as the (analytic) calculation of the inverse of the matrix \( (1 - R)^{-1} \) is needed.
3. Conclusions

The complex Langevin method presents a way to evade the sign problem in theories with complex actions. Promising recent developments have shown that it delivers very sensible results for QCD-like theories and even for full QCD. At small chemical potentials, where reweighting is feasible, the CL approach is validated by checking for agreement \[18\]. The theoretical foundation of the method in the case of a meromorphic action is not properly understood yet, but agreement with the systematic $\kappa$- and $\kappa_s$-expansions can be used to validate the method, by demonstrating that the poles cause no harm to the results.

These recent results show promise that the Complex Langevin approach will allow the exploration of the phase diagram of full QCD in detail, just as the phase diagram of HDQCD \[19\].

Acknowledgments – I thank to G. Aarts, F. Attanasio, Z. Fodor, B. Jäger, S.D. Katz, E. Seiler and I.-O. Stamatescu for discussions and collaboration on related work. Parts of the calculations were done on the bwGRiD (http://www.bw-grid.de), member of the German D-Grid initiative, funded by BMBF and MWFK Baden-Württemberg.

References

[1] P. de Forcrand, PoS LAT 2009 (2009) 010 [arXiv:1005.0539 [hep-lat]].
[2] G. Aarts, PoS LATTICE 2012 (2012) 017 [arXiv:1302.9028 [hep-lat]].
[3] E. Seiler, D. Sexty and I.-O. Stamatescu, Phys. Lett. B 723 (2013) 213 [arXiv:1211.3709 [hep-lat]].
[4] D. Sexty, Phys. Lett. B 729 (2014) 108 [arXiv:1307.7748 [hep-lat]].
[5] G. Aarts, Phys. Rev. Lett. 102 (2009) 131601 [arXiv:0810.2089 [hep-lat]].
[6] L. Bongiovanni, G. Aarts, E. Seiler, D. Sexty and I. O. Stamatescu, arXiv:1311.1056 [hep-lat].
[7] J. Berges and I.O. Stamatescu, Phys. Rev. Lett. 95 (2005) 202003 [hep-lat/0508030]. J. Berges, S. Borsanyi, D. Sexty and I.-O. Stamatescu, Phys. Rev. D 75 (2007) 045007 [hep-lat/0609058]. J. Berges and D. Sexty, Nucl. Phys. B 799 (2008) 306 [arXiv:0708.0779 [hep-lat]].
[8] G. Parisi, Phys. Lett. B 131 (1983) 393.
[9] J. R. Klauder, Stochastic quantization, in: H. Mitter, C.B. Lang (Eds.), Recent Developments in High-Energy Physics, Springer-Verlag, Wien, 1983, p. 351; J. Phys. A: Math. Gen. 16 (1983) L317; Phys. Rev. A 29 (1984) 2036.
[10] G. Aarts, E. Seiler and I.-O. Stamatescu, Phys. Rev. D 81 (2010) 054508 [arXiv:0912.3360 [hep-lat]].
[11] A. Mollgaard and K. Splittorff, Phys. Rev. D 88 (2013) 116007 [arXiv:1309.4335 [hep-lat]].
[12] G. Aarts, E. Seiler, D. Sexty and I. O. Stamatescu, arXiv:1408.3770 [hep-lat].
[13] G. Aarts, L. Bongiovanni, E. Seiler, D. Sexty and I.-O. Stamatescu, Eur. Phys. J. A 49 (2013) 89 [arXiv:1303.6425 [hep-lat]].
[14] G. Aarts, L. Bongiovanni, E. Seiler, D. Sexty and I.-O. Stamatescu, arXiv:1310.7412 [hep-lat].
[15] I. Bender et. al. Nucl. Phys. Proc. Suppl. 26 (1992) 323.
[16] T. D. Bakeyev and P. de Forcrand, Phys. Rev. D 63 (2001) 054505 [hep-lat/0008006]; G. Aarts, O. Kaczmarek, F. Karsch and I.-O. Stamatescu, Nucl. Phys. Proc. Suppl. 106 (2002) 456 [arXiv:hep-lat/0110145]; R. De Pietri, A. Feo, E. Seiler and I.-O. Stamatescu, Phys. Rev. D 76 (2007) 114501 [arXiv:0705.3420 [hep-lat]].
[17] M. Fromm, J. Langelage, S. Lottini and O. Philipsen, JHEP 1201 (2012) 042 [arXiv:1111.4953 [hep-lat]]; J. Greensite, J. C. Myers and K. Splittorff, Phys. Rev. D 88 (2013) 031502 [arXiv:1306.3085 [hep-lat]]; J. Langelage, M. Neuman and O. Philipsen, arXiv:1403.4162 [hep-lat].
[18] Z. Fodor, S.D. Katz, D. Sexty, in preparation.
[19] G. Aarts, F. Attanasio, B. Jäger, E. Seiler, I.-O. Stamatescu and D. Sexty, in preparation.