

Extending complex Langevin simulations to full QCD at nonzero density

Dénes Sexty*[†]

ITP, University of Heidelberg

E-mail: sexty.denes@gmail.com

Simulations of full QCD at nonzero baryon density using light quark masses are presented. The sign problem is evaded by the usage of the complex Langevin equation. The simulations are stabilized by the gauge cooling procedure for small lattice spacings. The method allows simulations at high densities, up to the saturation. The sign average is measured in the full as well as the phasequenched theory. Results are compared to the HQCD approach, in which the spatial hopping terms of fermionic variables are dropped, and good agreement is found at large masses.

31st International Symposium on Lattice Field Theory LATTICE 2013

July 29 - August 3, 2013

Mainz, Germany

*Speaker.

[†]I thank Gert Aarts, Erhard Seiler and Ion-Olimpiu Stamatescu for many discussions and collaboration on related work. A large part of the numerical calculations for this project was done on the bwGRiD (<http://www.bw-grid.de>), member of the German D-Grid initiative, funded by BMBF and MWFK Baden-Württemberg.

1. Introduction

The determination of the phase diagram of finite density QCD is one of the great problems of theoretical physics today. Lattice QCD is defined in terms of the euclidean path integral

$$Z = \int DU e^{-S_g[U]} \det M(\mu, U) \quad (1.1)$$

where $S_g[U]$ is the Yang-Mills action of the gauge fields and $M(\mu, U)$ is the Dirac-matrix of the quark fields. The well known sign problem prevents importance sampling simulations at $\mu \neq 0$, as the determinant of the fermion matrix is a complex number in this case. Various methods have been invented to circumvent the problem, but these are of limited use [1], mostly being applicable for $\mu/T \lesssim 1$. An exception is the complex Langevin method, which is not limited to small chemical potential. In this work I demonstrate that the algorithm can be successfully extended to full QCD with light quark masses on smooth lattices.

Shortly after the method of stochastic quantisation was proposed [2], it was noticed that it can be extended to complex actions [3]. The Langevin equation gets complexified and the variables are extended to a complexified manifold, which in the case of $SU(N)$ variables is $SL(N, \mathbb{C})$. The original theory is recovered for the averages of the analytically continued observables. This approach can be applied in many areas, for example for the real time path integral problem [4, 5, 6], or Yang-Mills theory with a Θ -term.

A recent approach also relying on the complexification of the variable space is the Lefschetz-thimble approach [7], where the path of the integration is shifted off the real axis in the complex plane to a path where the phase of the measure is constant. A residual sign problem is still present coming from the Jacobian of the transformation. This approach seems to be related to stochastic quantisation [8].

The complex Langevin method is known to sometimes produce convergent but wrong results, in other cases it solves theories with a severe sign problem. It has been tested for various systems inspired by finite-density QCD [9, 10, 11, 12, 13], in some cases unsuccessfully [14, 15, 16, 17, 18].

Although a complete understanding of the successes and breakdowns is still missing, our analytic understanding is improving steadily [19, 20, 21, 22, 23], and one can gain an insight whether the results are trustworthy using requirements such as the fast decay of the distributions.

Recently an important addition to the simulation algorithm of gauge theories called 'gauge cooling' was proposed [13, 24]. This procedure ensures that the distribution of the variables on the complex plane stays well localized, and this leads to correct results. It was shown that with this addition the simulation of an approximation to QCD called HQCD (in which spatial hoppings of fermions are dropped) can be successfully simulated [13], as well as full QCD with light quark masses [25].

2. The complex Langevin equation for lattice QCD

The discretised complex Langevin equation (CLE) for the link variables $U_{x,v}$ of lattice QCD with Langevin time step ε is written as

$$U_{x,v}(\tau + \varepsilon) = R_{x,v}(\tau) U_{x,v}(\tau), \quad (2.1)$$

with

$$R_{x,v}(\tau) = \exp \left[i \sum_a \lambda_a (\varepsilon K_{axv} + \sqrt{\varepsilon} \eta_{axv}) \right] \quad (2.2)$$

Here λ_a are the generators of the gauge group, i.e. the Gell-Mann matrices. The drift force is determined as

$$K_{axv} = -D_{axv} S_{\text{eff}}[U] \quad (2.3)$$

from the effective action $S_{\text{eff}}[U] = S_g[U] + \ln \det M[\mu, U]$ with the left derivative

$$D_a f(U) = \partial_{\alpha} f(e^{i\alpha \lambda_a} U) \Big|_{\alpha=0}. \quad (2.4)$$

In the case of QCD the drift term is written as

$$K_{axv} = -D_{axv} S_g[U] + \frac{N_F}{4} \text{Tr} [M^{-1}(\mu, U) D_{axv} M(\mu, U)]. \quad (2.5)$$

For the calculation of the fermionic drift the bilinear noise scheme is used [26, 27]. The numerical cost is therefore one CG solution for every update. The number of CG iterations needed for a given precision is highly dependent on the chemical potential, with larger μ requiring more iterations.

This Langevin update is interspersed with several gauge cooling updates, which make the simulation stable for not too small β parameter values [13, 25]. Typically the main cost of the simulation is the CG solution, the gauge force as well as the gauge cooling require less effort.

In the reweighting approach one defines the phasequenched theory

$$Z_{\text{pq}} = \int DU e^{-S_g[U]} |\det M(\mu, U)| = \int DU e^{-S_g[U]} \det M(\mu_I, U), \quad (2.6)$$

where the complex phase of the determinant is dropped. This change can also be understood physically if we introduce an isospin dependent chemical potential μ_I . We assume an even number of flavors. In this case isospin partners will have the opposite phase of the determinant, and the total determinant is positive, as written in eq. (2.6), making importance sampling possible. This theory can also be simulated with the Langevin equation, where the change to the full theory amounts to taking the real part of the drift force in the Langevin update. Gauge cooling is of course not needed in this case, one can reunitarize the link variables by hand to ensure they stay in the SU(3) group in spite of the numerical rounding errors.

In this work I use the Wilson plaquette action for the gauge fields with $N_F = 2$ or $N_F = 4$ flavors of unimproved staggered fermions.

3. Results

We are interested in the standard observables such as the Polyakov loop and inverse Polyakov loop

$$P = \frac{1}{V} \sum_x \text{Tr} P_x, \quad P' = \frac{1}{V} \sum_x \text{Tr} P_x^{-1} \quad \text{with} \quad P_x = \prod_{\tau=0}^{N_T-1} U_{(\tau,x),4}, \quad (3.1)$$

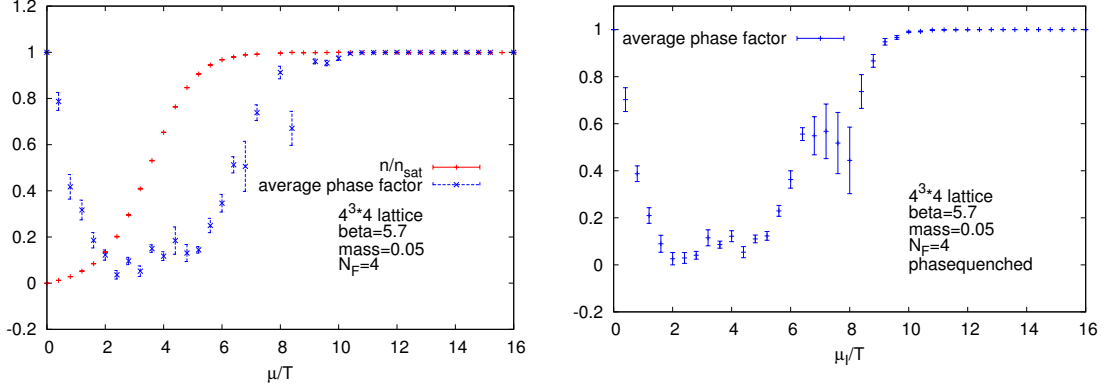


Figure 1: On the left panel the average phase factor and density is shown as a function of the chemical potential. On the right panel the average phase factor in the phasequenched theory is shown.

the chiral condensate

$$\langle \Psi^\dagger(x)\Psi(x) \rangle = \langle \partial \ln Z / \partial m \rangle / \Omega, \quad (3.2)$$

with $\Omega = V/T$ the space-time volume, and the density of the fermions

$$\langle n \rangle = \frac{1}{\Omega} \frac{\partial \ln Z}{\partial \mu}, \quad (3.3)$$

measured in units of the saturation density. The average phase factor of the determinant is defined as

$$\langle e^{2i\phi} \rangle = \left\langle \frac{\det M(\mu)}{\det M(-\mu)} \right\rangle. \quad (3.4)$$

This gives an impression of the distribution of the phases of the determinant. The average phase factor measured in the phasequenched theory is a direct indicator of the severeness of the sign-problem.

In Fig. 1 the density of the fermions as well as the average phase factor is shown. A small lattice is used as the direct calculation of the determinant is very costly. The parameters are such that the high temperature phase is tested, well above the phase transition (which is around $\beta_c \approx 5.04$ for the parameters used). Therefore the density starts to increase right away, as there are available excitations in the plasma. This is in contrast to the low temperature Silver Blaze behavior, where the chemical potential must reach a threshold before anything happens [28, 29]. At high chemical potentials the saturation is reached, where all available fermionic states are filled. Note that the average phase factor is close to zero in a large region of chemical potentials in the full as well as the phasequenched theory. This makes the reweighting approach in this range of chemical potentials unfeasible.

Fermionic observables as well as the Polyakov loops are measured at a fixed temperature as a function of the chemical potential in Fig. 2. One observes the expected behavior of the Polyakov loops: as the fermionic density increases, they grow as the system gets more ordered. The inverse Polyakov loop peaks before the Polyakov loop [13]. Eventually, in the saturation region the Polyakov loops have to vanish, as the fermions have no influence on the system, and the Z_3 symmetry is restored. This is also reflected in the bigger fluctuations of the Polyakov loops.

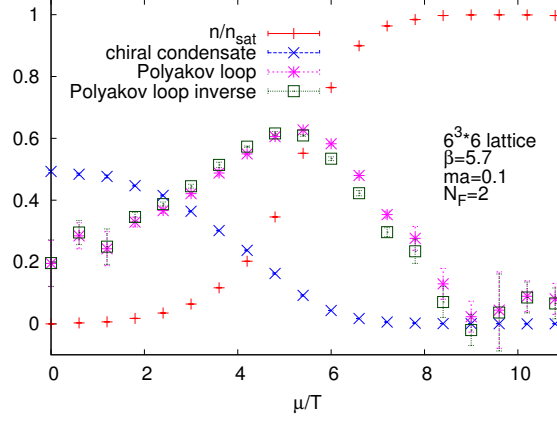


Figure 2: The fermion density, the chiral condensate and the trace of the Polyakov loop and its inverse as a function of the chemical potential.

3.1 Comparison with HQCD

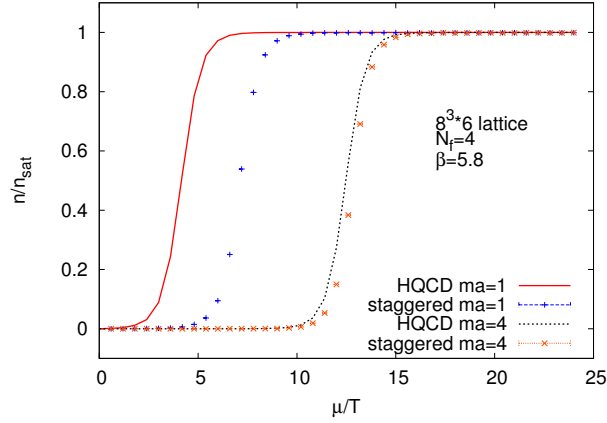


Figure 3: Comparison of the average densities measured in HQCD and in full QCD with staggered fermions.

A well known approximation to full QCD at high quark masses and large chemical potentials is the Heavy Quark QCD (HQCD) [30, 31]. In this approach the spatial hoppings are neglected, as they give a subleading contribution. The determinant simplifies to

$$\det(M(\mu, U)) = \prod_x \det(1 + CP_x) \det(1 + C'P_x^{-1}) \quad (3.5)$$

with the Polyakov loop (3.1) and the parameters $C = e^{\mu N_T} / (2m)^{N_T}$ and $C' = e^{-\mu N_T} / (2m)^{N_T}$ with the staggered mass m . A similar approximation can also be carried out for Wilson fermions, which was studied with the CLE in [13].

At large masses one can test the quality of the HQCD approximation by comparing it to full QCD. In Fig. 3 the fermion density is compared, in Fig. 4, the Polyakov loops and the spatial plaquette variables are compared.

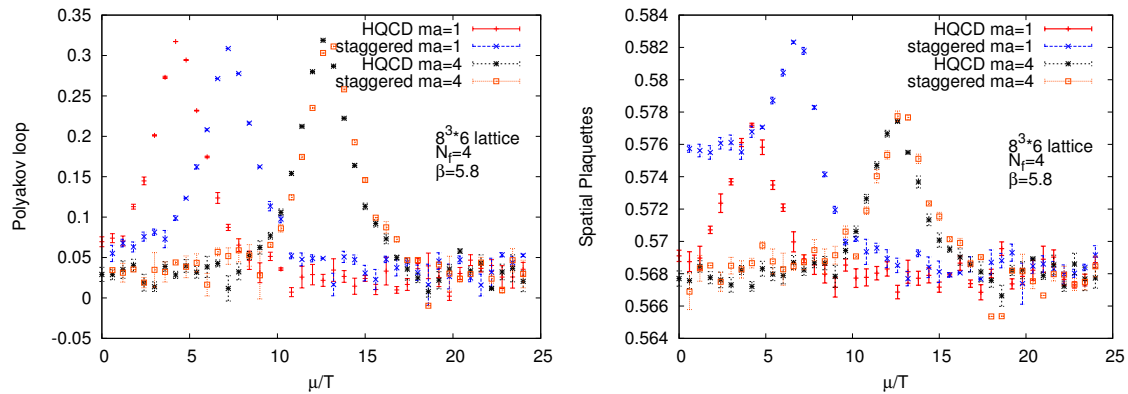


Figure 4: Comparison of the average Polyakov loops (left) and average spatial plaquettes (right) measured in HQCD and in full QCD with staggered fermions.

One notes that at $m = 4$ the agreement becomes quantitatively good, but the qualitative behavior is similar already at smaller mass, with a 'rescaled' chemical potential. This does not prove that the results are fully reliable, but the HQCD approach has been validated with reweighting at small μ , therefore it increases confidence that the CLE supplies correct results in this case.

4. Conclusions

The complex Langevin equation has been applied to full QCD at non-zero density. The simulations are controlled using the gauge cooling procedure for not too big lattice spacings. The method allows calculations at arbitrary densities all the way up to saturation. There is no sign or overlap problem in complex Langevin simulations, the non-positiveness of the measure is taken into account by the analytic continuation of the variables to the complexified manifold $SL(3, \mathbb{C})$. The method allows simulations of full QCD with light fermions at high densities for the first time.

The procedure gives the physically expected results, the saturation physics at large chemical potentials and the expected behavior of the Polyakov loops and inverse Polyakov loops is correctly reproduced. To further increase confidence in the method, the next check would be to compare the full theory with the phasequenched one at low temperatures, where the onset of the density has to reflect the crucial difference between the two theories.

References

- [1] P. de Forcrand, PoS LAT **2009**, 010 (2009) [arXiv:1005.0539]; G. Aarts, PoS LATTICE **2012** (2012) 017 [arXiv:1302.3028].
- [2] G. Parisi and Y. -s. Wu, Sci. Sin. **24** (1981) 483.
- [3] G. Parisi, Phys. Lett. **131 B** (1983) 393.
- [4] J. Berges and I. -O. Stamatescu, Phys. Rev. Lett. **95** (2005) 202003 [hep-lat/0508030].
- [5] J. Berges, S. .Borsanyi, D. Sexty and I. -O. Stamatescu, Phys. Rev. D **75** (2007) 045007 [hep-lat/0609058].

- [6] J. Berges and D. Sexty, Nucl. Phys. B **799** (2008) 306 [arXiv:0708.0779].
- [7] M. Cristoforetti *et al.* [AuroraScience Collaboration], Phys. Rev. D **86** (2012) 074506 [arXiv:1205.3996 [hep-lat]]; M. Cristoforetti, L. Scorzato and F. Di Renzo, J. Phys. Conf. Ser. **432** (2013) 012025 [arXiv:1210.8026 [hep-lat]].
- [8] G. Aarts, arXiv:1308.4811 [hep-lat].
- [9] G. Aarts and I. -O. Stamatescu, JHEP **0809** (2008) 018 [arXiv:0807.1597].
- [10] G. Aarts, Phys. Rev. Lett. **102** (2009) 131601 [arXiv:0810.2089 [hep-lat]].
- [11] G. Aarts and K. Splittorff, JHEP **1008**, 017 (2010) [arXiv:1006.0332 [hep-lat]].
- [12] G. Aarts and F. A. James, JHEP **1201** (2012) 118 [arXiv:1112.4655].
- [13] E. Seiler, D. Sexty and I. -O. Stamatescu, Phys. Lett. B **723**, 213 (2013) [arXiv:1211.3709 [hep-lat]].
- [14] J. Ambjorn and S. K. Yang, Phys. Lett. B **165**, 140 (1985).
- [15] J. Ambjorn, M. Flensburg and C. Peterson, Nucl. Phys. B **275**, 375 (1986).
- [16] G. Aarts and F. A. James, JHEP **1008** (2010) 020 [arXiv:1005.3468].
- [17] J. M. Pawłowski and C. Zielinski, Phys. Rev. D **87**, 094509 (2013) [arXiv:1302.2249 [hep-lat]]; J. M. Pawłowski and C. Zielinski, Phys. Rev. D **87**, 094503 (2013) [arXiv:1302.1622 [hep-lat]].
- [18] A. Mollgaard and K. Splittorff, arXiv:1309.4335 [hep-lat].
- [19] G. Aarts, E. Seiler and I. -O. Stamatescu, Phys. Rev. D **81** (2010) 054508 [arXiv:0912.3360]; G. Aarts, F. A. James, E. Seiler and I. -O. Stamatescu, Eur. Phys. J. C **71** (2011) 1756 [arXiv:1101.3270].
- [20] C. Pehlevan and G. Guralnik, Nucl. Phys. B **811** (2009) 519 [arXiv:0710.3756]; G. Guralnik and C. Pehlevan, Nucl. Phys. B **822** (2009) 349 [arXiv:0902.1503].
- [21] G. Aarts, F. A. James, J. M. Pawłowski, E. Seiler, D. Sexty and I. -O. Stamatescu, JHEP **1303**, 073 (2013) [arXiv:1212.5231 [hep-lat]].
- [22] A. Duncan and M. Niedermaier, Annals Phys. **329**, 93 (2013).
- [23] G. Aarts, P. Giudice and E. Seiler, arXiv:1306.3075 [hep-lat].
- [24] G. Aarts, L. Bongiovanni, E. Seiler, D. Sexty and I. -O. Stamatescu, arXiv:1303.6425 [hep-lat].
- [25] D. Sexty, arXiv:1307.7748 [hep-lat].
- [26] G. G. Batrouni, G. R. Katz, A. S. Kronfeld, G. P. Lepage, B. Svetitsky and K. G. Wilson, Phys. Rev. D **32** (1985) 2736.
- [27] M. Fukugita, Y. Oyanagi and A. Ukawa, Phys. Rev. D **36** (1987) 824.
- [28] T. D. Cohen, Phys. Rev. Lett. **91** (2003) 222001 [hep-ph/0307089].
- [29] M. Fromm, J. Langelage, S. Lottini and O. Philipsen, JHEP **1201** (2012) 042 [arXiv:1111.4953]; M. Fromm, J. Langelage, S. Lottini, M. Neuman and O. Philipsen, arXiv:1207.3005 [hep-lat].
- [30] I. Bender, T. Hashimoto, F. Karsch, V. Linke, A. Nakamura, M. Plewnia, I. O. Stamatescu and W. Wetzel, Nucl. Phys. Proc. Suppl. **26** (1992) 323; T. C. Blum, J. E. Hetrick and D. Toussaint, Phys. Rev. Lett. **76** (1996) 1019 [hep-lat/9509002].
- [31] R. De Pietri, A. Feo, E. Seiler and I. -O. Stamatescu, Phys. Rev. D **76** (2007) 114501 [arXiv:0705.3420].