Complex Langevin dynamics in the SU(3) spin model at nonzero chemical potential

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ABSTRACT

The three-dimensional SU(3) spin model is an effective Polyakov loop model for QCD at nonzero temperature and density. It suffers from a sign problem at nonzero chemical potential. We revisit this model using complex Langevin dynamics and assess in particular the justification of this approach, using analyticity at small μ^2, an effective toy model and the criteria for correctness developed recently. Our results strongly indicate that complex Langevin dynamics is reliable in this theory in both phases, including the critical region. This is in sharp contrast to the case of the XY model, where correct results were obtained in only part of the phase diagram.

1 Introduction

1.1 Complex actions and the sign problem

- Field theories with a complex action difficult to treat nonperturbatively because the weight in the path integral is not positive

$$Z = \int D\phi\, e^{-S} = \int D\phi\, \left|e^{-S}\right| e^{i\varphi}, \tag{1}$$

- Known as the **sign problem**
- Main issue preventing a fully nonperturbative study of the QCD phase diagram.
- One possibility: absorb the phase into the observable and reweight with respect to the real and postive weight, called the **phase quenched** approximation,

$$\langle O\rangle = \frac{\int D\phi\, O(\phi) e^{i\varphi}\left|e^{-S}\right|}{\int D\phi\, e^{i\varphi}\left|e^{-S}\right|} = \frac{\langle O e^{i\varphi}\rangle_{\rm pq}}{\langle e^{i\varphi}\rangle_{\rm pq}}. \tag{2}$$

- Overlap between the correct and phase quenched weights becomes very small in the limit of either large volume Ω or chemical potential,

$$\langle e^{i\varphi}\rangle_{\rm pq} = \frac{\int D\phi \left|e^{-S}\right| e^{i\varphi}}{\int D\phi \left|e^{-S}\right|} = \frac{Z}{Z_{\rm pq}} \sim e^{-\Omega\Delta f}, \tag{3}$$

1.2 Complex Langevin dynamics

- Langevin dynamics does not rely on importance sampling
- Add extra time-like parameter, ϑ, and evolve variables ϕ, with Gaussian noise kick η according to Langevin equation

$$\frac{\partial\phi}{\partial\vartheta} = K + \eta, \qquad K = -\frac{\delta S}{\delta\phi}. \tag{4}$$

- Expectation values from noise averages in infinite time limit

$$\langle O\rangle = \lim_{\vartheta\to\infty}\langle O\rangle_\eta. \tag{5}$$

- With complex action, extend degrees of freedom $\phi \to \phi^{\rm R} + i\phi^{\rm I}$, gives complex Langevin equation

$$\frac{\partial\phi^{\rm R}}{\partial\vartheta} = {\rm Re}\ K(\phi)\Big|_{\phi\to\phi^{\rm R}+i\phi^{\rm I}} + \eta, \qquad \frac{\partial\phi^{\rm I}}{\partial\vartheta} = {\rm Im}\ K(\phi)\Big|_{\phi\to\phi^{\rm R}+i\phi^{\rm I}}. \tag{6}$$

- Known problems with complex Langevin dynamics include numerical instabilities and incorrect convergence [1].
- Numerical instabilities can be cured with an adaptive stepsize [2], incorrect convergence a more pressing problem (addressed here)

2 Overview and background

2.1 SU(3) spin model

- Effective Polyakov loop model which follows from QCD in a combined strong-coupling and heavy-quark expansion.
- One of the first QCD-related models to be studied with complex Langevin dynamics [3],
- Has action $S = S_B + S_F$,

$$S_B = -\beta\sum_{x,\nu} {\rm Tr}\, U_x {\rm Tr}\, U^\dagger_{x+\hat\nu} + {\rm Tr}\, U^\dagger_x {\rm Tr}\, U_{x+\hat\nu}, \tag{7}$$

$$S_F = -h\sum_x \left(e^\mu {\rm Tr}\, U_x + e^{-\mu}{\rm Tr}\, U^\dagger_x\right). \tag{8}$$

- Diagonalise,

$${\rm Tr}\, U = e^{i\phi_1} + e^{i\phi_2} + e^{-i(\phi_1+\phi_2)}, \tag{9}$$

$${\rm Tr}\, U^\dagger = e^{-i\phi_1} + e^{-i\phi_2} + e^{i(\phi_1+\phi_2)}. \tag{10}$$

- Extra term S_H from Haar measure,

$$S_H = -\sum_x \ln\left[\sin^2\left(\frac{\phi_{1,x}-\phi_{2,x}}{2}\right)\sin^2\left(\frac{2\phi_{1,x}+\phi_{2,x}}{2}\right)\sin^2\left(\frac{\phi_{1,x}+2\phi_{2,x}}{2}\right)\right] \tag{11}$$

- At small h, disordered phase at small β seperated from an ordered phase at larger β by a 1st order transition, which weakens to a crossover ending in a critital end point for larger chemical potentials

2.2 Improved algorithm

- Numerical solution to Langevin equation converges to weight with stepsize corrections,

$$P[\phi] = e^{-\bar S} = e^{-(S_0+\epsilon S_1+\ldots)} \tag{12}$$

- Improved integration algorithm [4] reduces stepsize corrections from $O(\epsilon)$ to $O(\epsilon^{3/2})$
- Add extra intermediate points $\psi, \tilde\psi$ and use the update rule

$$\psi_{ax}(n) = \phi_{ax}(n) + \frac{1}{2}\epsilon K[\phi_{ax}(n)], \tag{13}$$

$$\tilde\psi_{ax}(n) = \phi_{ax}(n) + \frac{1}{2}\epsilon K[\phi_{ax}(n)] + \frac{3}{2}\sqrt{\epsilon}\tilde\alpha_{ax}(n), \tag{14}$$

$$\phi_{ax}(n+1) = \phi_{ax}(n) + \frac{1}{3}\epsilon\left(K[\psi_{ax}(n) + 2K[\tilde\psi_{ax}(n)]\right) + \sqrt{\epsilon}\alpha_{ax}(n), \tag{15}$$

- With $\tilde\alpha$ composed of Gaussian random numbers α, ξ

$$\tilde\alpha_{ax}(n) = \frac{1}{2}\alpha_{ax}(n) + \frac{\sqrt{3}}{6}\xi_{ax}(n), \tag{16}$$

$$\langle\alpha_{ax}(n)\alpha_{by}(m)\rangle = \langle\xi_{ax}(n)\xi_{by}(m)\rangle = \delta_{ab}\delta_{xy}\delta_{mn}, \tag{17}$$

$$\langle\alpha_{ax}(n)\xi_{by}(m)\rangle = \langle\alpha_{ax}(n)\rangle = \langle\xi_{ax}(n)\rangle = 0. \tag{18}$$

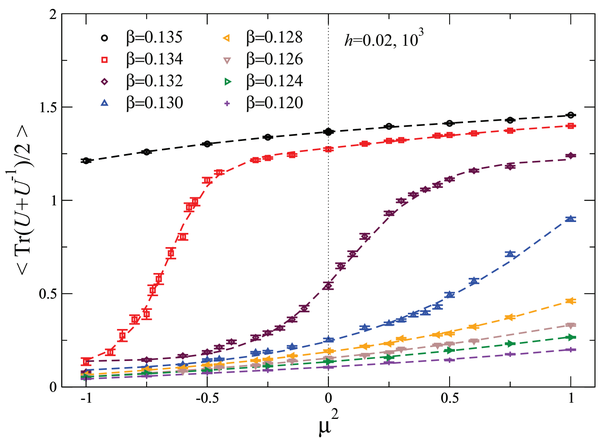
3 Results

3.1 Imaginary chemical potential

- Take imaginary chemical potential, $\mu = i\mu_I$.

$$S_F(\mu) = \sum_x {\rm Tr}\, U_x e^{i\mu} + {\rm Tr}\, U^\dagger_x e^{-i\mu} = [S_F(\mu)]^\dagger, \tag{19}$$

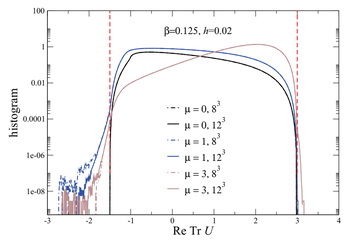
- Action becomes real and can use standard Monte Carlo techniques
- Observables even in μ should be continuous between imaginary and real chemical potential results.

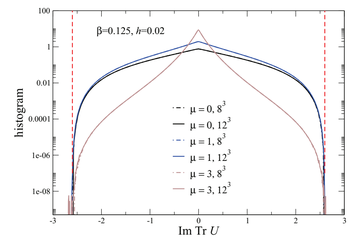


3.2 Distributions

- Compute distribution of observables during Langevin evolution
- Sample from complex plane, observables rarely go outside the real limits

$$-\frac{3}{2} \le {\rm Re\,Tr}\, U \le 3, \qquad -\frac{3\sqrt{3}}{2} \le {\rm Im\,Tr}\, U \le \frac{3\sqrt{3}}{2}, \tag{20}$$

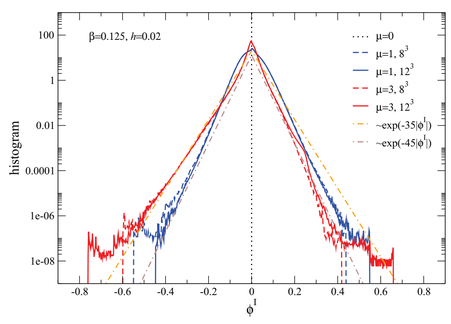




- Need decay of distribution in imaginary direction $P[\phi^{\rm I}]$ to be sufficiently fast for integration

$$\int D\phi^{\rm R} D\phi^{\rm I}\, O(\phi^{\rm R} + i\phi^{\rm I}) P[\phi^{\rm R}, \phi^{\rm I}] \tag{21}$$

- Histogram shows decay is $P[\phi^{\rm I}] \sim e^{-c|\phi^{\rm I}|}$, with $c \sim 40$ so potential problem for observables like $O = {\rm Tr}\, U^k$ with $k \gtrsim 40$
- Contributions of the form $e^{ik\phi} = e^{-k\phi^{\rm I}}\cos(k\phi^{\rm R})$ so rapidly oscillating cosine should be taken into account.



3.3 Criteria and stepsize extrapolation

- Instead of considering Langevin dynamics and noise averages, can instead use dual Fokker-Planck equation and probability distribution $P[\phi^{\rm R}, \phi^{\rm I}; \vartheta]$,

$$\frac{\partial}{\partial\vartheta}P[\phi^{\rm R}, \phi^{\rm I}; \vartheta] = \left[\frac{\partial}{\partial\phi^{\rm R}}\left(\frac{\partial}{\partial\phi^{\rm R}} - K^{\rm R}\right) - \frac{\partial}{\partial\phi^{\rm I}}K^{\rm I}\right]P[\phi^{\rm R}, \phi^{\rm I}; \vartheta], \tag{22}$$

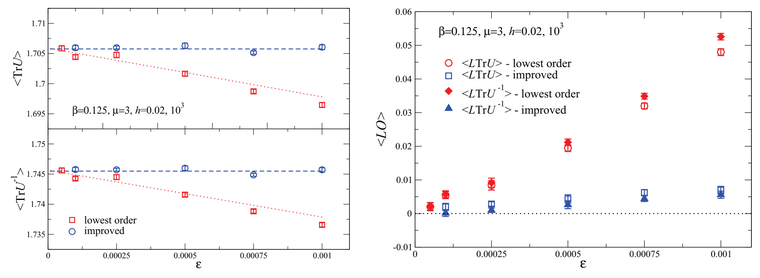
- Expectation values taken with respect to real and positive equilibrium distribution

$$\langle O\rangle = \int D\phi^{\rm R} D\phi^{\rm I}\, O(\phi^{\rm R} + i\phi^{\rm I}) P[\phi^{\rm R}, \phi^{\rm I}; \infty], \tag{23}$$

- Can compare the time evolution of probability distribution $P[\phi^{\rm R}, \phi^{\rm I}; \vartheta]$ and a complex density that represents the original problem $\rho[\phi; \vartheta]$
- Arrive at a necessary condition for correct results [5] which requires that for all observables $\langle LO(\phi)\rangle$ vanishes, with the operator

$$L = \frac{\partial}{\partial\phi}\left(\frac{\partial}{\partial\phi} - K\right)O(\phi) \tag{24}$$

- Simulations with SU(3) spin model show $\langle {\rm Tr}\, U\rangle$ vanishes as $\epsilon \to 0$



4 Effective 1-link model

- Rewrite action to focus on single lattice site, viewing neighbour interactions as coupling to external complex parameter

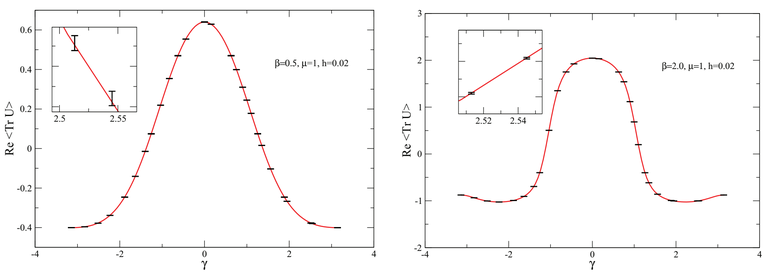
$$S_B = -\beta\sum_x\Big[\,{\rm Tr}\, U_x\left(\sum_\nu {\rm Tr}\, U^\dagger_{x+\hat\nu} + {\rm Tr}\, U^\dagger_{x-\hat\nu}\right) + {\rm Tr}\, U^\dagger_x\left(\sum_\nu {\rm Tr}\, U_{x+\hat\nu} + {\rm Tr}\, U_{x-\hat\nu}\right)\Big]. \tag{25}$$

- Motivates the toy model of a single site with parameters β, γ

$$\beta_1 = \beta e^{i\gamma} + he^{\mu}, \qquad \beta_2 = \beta e^{-i\gamma} + he^{-\mu}, \tag{26}$$

$$S = -\beta_1 {\rm Tr}\, U - \beta_2 {\rm Tr}\, U^\dagger, \tag{27}$$

- Find that complex Langevin dynamics gives correct results for all complex parameters
- Follows that the full lattice model must also work correctly.



5 Conclusions

To ascertain whether the complex Langevin process is converging to the correct distribution we have applied a range of different tests and find that all results are consistent with correct convergence. These tests show

- Imaginary chemical potential analyticity across $\mu^2 = 0$
- Distributions of observables and $\phi^{\rm I}$ narrow and decay fast
- Criteria for correctness vanish as $\epsilon \to 0$
- Effective 1-link toy model works correctly for all complex parameters

The improved integration scheme reduces stepsize effects from $O(\epsilon)$ to $O(\epsilon^{3/2})$ and therefore allows much larger stepsizes to be used.

References

[1] G. Aarts, E. Seiler, I. -O. Stamatescu, Phys. Rev. **D81** (2010) 054508 [arXiv:0912.3360 [hep-lat]].

[2] G. Aarts, F. A. James, E. Seiler and I. -O. Stamatescu, Phys. Lett. B **687** (2010) 154 [arXiv:0912.0617 [hep-lat]].

[3] F. Karsch and H. W. Wyld, Phys. Rev. Lett. **55** (1985) 2242.

[4] Chein-Cheng-Chang, Math. Comp. **49** 180 (1987) 523-542.

[5] G. Aarts, F. A. James, E. Seiler, I. -O. Stamatescu, Eur. Phys. J. **C71** (2011) 1756 [arXiv:1101.3270 [hep-lat]].

[6] G. Aarts and F. A. James, JHEP **1201** (2012) 118 [arXiv:1112.4655 [hep-lat]].