Complex Langevin dynamics: an overview of recent developments

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Outline

- Introduction to complex Langevin dynamics
- Formal arguments for correct convergence
- Criteria for correctness
- An improved integration algorithm
- Study of SU(3) spin model with chemical potential

Introduction

- Goal: lattice simulations to determine QCD phase structure
- Problem: chemical potential makes action complex
- Complex weight can't be interpreted as a probability

$$Z = \int D\phi \left| e^{-S(\phi)} \right| e^{i\varphi}$$

- Standard methods based on importance sampling break down
- Origin of the sign problem

Reweighting

- Can shift complex phase from weight to observable
- Simulate with respect to a real and positive weight, phase quenched theory

$$\langle O \rangle = \frac{\int D\phi \, O(\phi) e^{i\varphi} |e^{-S(\phi)}|}{\int D\phi \, e^{i\varphi} |e^{-S(\phi)}|} = \frac{\langle O e^{i\varphi} \rangle_{\mathrm{pq}}}{\langle e^{i\varphi} \rangle_{\mathrm{pq}}}$$

- Problem: the phase vanishes exponentially as volume $\Omega \to \infty$:

$$\langle e^{i\varphi} \rangle_{\mathrm{pq}} = \frac{Z}{Z_{\mathrm{pq}}} \sim e^{-\Omega \Delta f}$$

- Required simulation time grows expontentially
- Can measure $\langle e^{i\varphi} \rangle_{\mathrm{pq}}$ to quantify "severeness" of sign problem

Langevin dynamics

- Langevin dynamics does not rely on importance sampling
- Add fictitious time-like parameter ϑ (Langevin time), $\phi \to \phi(\vartheta)$
- Equation of motion with noise term, Langevin equation

$$\frac{\partial \phi}{\partial \vartheta} = -\frac{\delta S(\phi)}{\delta \phi} + \eta$$

- Fluctuations from Gaussian noise

$$\langle \eta(\vartheta)\eta(\vartheta')\rangle = 2\delta(\vartheta - \vartheta'), \qquad \langle \eta(\vartheta)\rangle = 0$$

Expectation values

- Expectation values taken as noise averages
- Equal to quantum expectation values in limit of large times

$$\lim_{\vartheta \to \infty} \langle O(\vartheta) \rangle_\eta = \langle O \rangle$$

- When action is real, can be shown that the stationary solution generates configurations distributed e^{-S}

Complex Langevin dynamics

- With action complex, can still write down the (complex) Langevin equation
- Complex drift term forces all degrees of freedom into complex plane
- Need to complexify degrees of freedom $\phi \to \phi^{\mathrm{R}} + i\phi^{\mathrm{I}}$,

$$\frac{\partial \phi^{\mathrm{R}}}{\partial \vartheta} = K^{\mathrm{R}} + \eta, \qquad \frac{\partial \phi^{\mathrm{I}}}{\partial \vartheta} = K^{\mathrm{I}}$$

- Drift terms given by

$$K^{\mathrm{R}} = -\mathrm{Re}\,\frac{\delta S}{\delta \phi}\bigg|_{\phi \to \phi^{\mathrm{R}} + i\phi^{\mathrm{I}}}, \qquad K^{\mathrm{I}} = -\mathrm{Im}\,\frac{\delta S}{\delta \phi}\bigg|_{\phi \to \phi^{\mathrm{R}} + i\phi^{\mathrm{I}}}$$

Discretised equations

- Discretise time: $\vartheta = \epsilon n$
- Standard (Euler) integration:

$$\phi^{\mathrm{R}}(n+1) = \phi^{\mathrm{R}}(n) + \epsilon K^{\mathrm{R}}(n) + \sqrt{\epsilon}\eta(n)$$
$$\phi^{\mathrm{I}}(n+1) = \phi^{\mathrm{I}}(n) + \epsilon K^{\mathrm{I}}(n)$$

- Introduces $O(\epsilon)$ stepsize corrections
- Discrete process generates configurations distributed with effective action

$$\bar{S} = S_0 + \epsilon S_1 + \ldots$$

- Correct results obtained by extrapolation to $\epsilon \to 0$

A simple example

- Single degree of freedom:

$$S = \frac{1}{2}\sigma x^2, \qquad \sigma = A + iB$$

- Complexify $x \to x + iy$ and get Langevin equations

$$\dot{x} = K_x + \eta, \qquad \dot{y} = K_y$$

- Force terms

$$K_x = -Ax + By, \qquad K_y = -Ay - Bx$$

- Can solve the equation of motion directly, taking initial conditions $x(0) = y(0) = 0$:

$$x(\vartheta) = \int_0^{\vartheta} e^{-A(\vartheta - s)} \cos[B(\vartheta - s)]\eta(s)ds$$

$$y(\vartheta) = -\int_0^{\vartheta} e^{-A(\vartheta - s)} \sin[B(\vartheta - s)]\eta(s)ds$$

A simple example

- Expectation values in limit $\vartheta \to \infty$

$$\langle x^2 \rangle = \frac{1}{2A} \frac{2A^2 + B^2}{A^2 + B^2}$$
$$\langle y^2 \rangle = \frac{1}{2A} \frac{B^2}{A^2 + B^2}$$
$$\langle xy \rangle = -\frac{1}{2} \frac{B}{A^2 + B^2}$$

- The correct (holomorphic) combination is recovered

$$\langle x^2 \rangle \to \langle x^2 - y^2 + 2ixy \rangle = \frac{A - iB}{A^2 + B^2} = \frac{1}{A + iB} = \frac{1}{\sigma}$$

What is the problem?

- Looks good: simple idea, easy to implement and known about since 1980s
- Some problems:
  - New degree of freedom ϕ^{I} is unbounded
  - Simulations can be unstable and follow runaway trajectories in direction ϕ^{I}
  - No proof of convergence to correct distribution (or at all)
  - Simulations can converge to a well defined distribution, but results turn out to be wrong Aarts, FJ, 2010
- Instabilities cured by careful integration with an adaptive stepsize Aarts, FJ, Seiler, Stamatescu, 2010

Formal arguments

- Aim: understand conditions for correct convergence of complex Langevin process Aarts, FJ, Seiler, Stamatescu 2011
- For simplicity, consider a single degree of freedom, x
- Replace original measure with the equilibrium distribution P of the complex Langevin process
  1. Complex measure $e^{-S}dx$, which suffers from a sign problem
  2. Real and positive measure $Pdxdy$, complex Langevin solution
- Expectation values of holomorphic functions should agree

Fokker-Planck equation

- Fokker-Planck equation dual to complex Langevin process

$$\frac{\partial}{\partial \vartheta} P(x, y; \vartheta) = L^T P(x, y; \vartheta)$$

- Fokker-Planck operator given by

$$L^T = \nabla_x [\nabla_x - K_x] - \nabla_y K_y$$

- $P(x, y; \vartheta)$ is a real distribution
- Probability density of at time ϑ for the complexified variables x, y

Complex Fokker-Planck equation

- Also consider the complex density $\rho(x;\vartheta)$ with x real

$$\frac{\partial}{\partial\vartheta}\rho(x;\vartheta) = L_0^T \rho(x;\vartheta)$$

- Complex Fokker-Planck operator

$$L_0^T = \nabla_x[\nabla_x + (\nabla_x S(x))]$$

- Complex density represents original description, suffers from sign problem
- Correct stationary solution for ρ exists

$$\rho(x;\infty) \propto e^{-S(x)}$$

Evolution of the densitities

- Define expectation values

$$\langle O \rangle_{P(\vartheta)} = \frac{\int O(x+iy)P(x,y;\vartheta)dxdy}{\int P(x,y;\vartheta)dxdy}$$

$$\langle O \rangle_{\rho(\vartheta)} = \frac{\int O(x)\rho(x;\vartheta)dx}{\int \rho(x;\vartheta)dx}$$

- Need to show that expecation values match

$$\langle O \rangle_{P(\vartheta)} = \langle O \rangle_{\rho(\vartheta)}$$

- Initial conditions match requires

$$P(x,y;0) = \rho(x;0)\delta(y)$$

Shifting time dependence

- Shift time dependence from densities to observable
- On holomorphic observables, may act with Langevin operator

$$\tilde{L} = [\nabla_x - (\nabla_x S(x))]\nabla_x$$

- Action of $\tilde{L}$ on holomorphic functions agrees with that of L
- Evolution of observables given by

$$\frac{\partial}{\partial \vartheta} O(x; \vartheta) = \tilde{L} O(x; \vartheta)$$

- Formally solved by

$$O(x; \vartheta) = \exp(\vartheta \tilde{L}) O(x)$$

Conditions for correct results

- Consider

$$F(\vartheta, \vartheta') = \int P(x, y; \vartheta - \vartheta') O(x + iy; \vartheta') dxdy$$

- Interpolates between the two expectation values

$$F(\vartheta, 0) = \int P(x, y; \vartheta) O(x + iy; 0) dxdy = \langle O \rangle_{P(\vartheta)}$$

$$\begin{aligned} F(\vartheta, \vartheta) &= \int P(x, y; 0) O(x + iy; \vartheta) dxdy \\ &= \int \rho(x; 0) \left(e^{\vartheta L_0} O \right) (x; 0) dx \\ &= \int O(x; 0) \left(e^{\vartheta L_0^T} \rho \right) (x; 0) dx \\ &= \langle O \rangle_{\rho(\vartheta)} \end{aligned}$$

Integration by parts

- Expectation values match if $F(\vartheta, \vartheta')$ independent of ϑ:

$$\frac{\partial}{\partial \vartheta'} F(\vartheta, \vartheta') = -\int (L^T P(x, y; \vartheta - \vartheta')) O(x + iy; \vartheta') dxdy + \int P(x, y; \vartheta - \vartheta') L O(x + iy; \vartheta') dxdy$$

- Integration by parts gives required cancellation

$$\int P(x, y; \vartheta - \vartheta') L O(x + iy; \vartheta') dxdy \rightarrow \int L^T P(x, y; \vartheta - \vartheta') O(x + iy; \vartheta') dxdy$$

- Needs boundary terms to vanish for $\langle O \rangle_\rho = \langle O \rangle_P$

Boundary terms

- Vanishing boundary terms requires decay of distribution to be sufficiently fast
- Products of observable and distribution (and derivatives)

$$P(x, y; \vartheta - \vartheta')O(x + iy; \vartheta')$$

- Real direction x will be either compact or distribution rapidly decaying
- Need distribution "narrow" and fast decay in imaginary direction y

Criteria for correctness

- Take slightly weaker condition $\vartheta' = 0$ and $\vartheta \to \infty$
- Condition now becomes

$$\frac{\partial}{\partial \vartheta'} F(\infty, \vartheta')\Big|_{\vartheta'=0} = -\int (L^T P(x, y, \infty)) O(x+iy, 0) dxdy + \int P(x, y, \infty) L O(x+iy, 0) dxdy$$

- First term vanishes automatically due to

$$L^T P(x, y; \infty) = 0$$

- Therefore ϑ'-independence requires

$$\langle LO \rangle = \int P(x, y; \infty) L O(x+iy; 0) dxdy = 0$$

- Can be checked for any given observable
- Stong statement: should be true for all observables

SU(3) spin model

- Effective dimensionally reduced polyakov loop model for QCD
- Studied using complex Langevin dynamics in 1980s

  Karsh and Wyld, 1985
- Recently developed method using flux formalism to circumvent sign problem in an alternate way Gattringer 2011
- Action given by $S = S_B + S_F$,

$$S_B = -\beta \sum_x \sum_{\nu=1}^{3} \mathrm{Tr}\, U_x \mathrm{Tr}\, U^\dagger_{x+\hat{\nu}} + \mathrm{Tr}\, U_{x+\hat{\nu}} \mathrm{Tr}\, U^\dagger_x$$

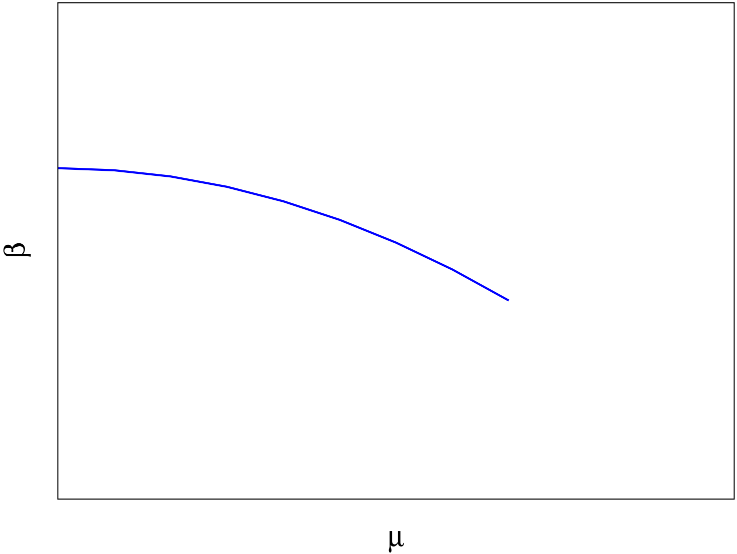
$$S_F = -h \sum_x e^{\mu} \mathrm{Tr}\, U_x + e^{-\mu} \mathrm{Tr}\, U^\dagger_x$$

- Contribution S_F makes action complex when $\mu \neq 0$, sign problem

Phase structure

- Phase transition in region of small h
- Disordered (confined) phase for lower β values
- Ordered (deconfined) phase for higher β values
- Phases seperated by a first-order transition
- Increasing chemical potential weakens the transition and becomes a crossover at a critial point
- At larger h there is a crossover only

Phase structucture with small h



Langevin equations

- Can diagonalise U_x, write in terms of angles

$$\mathrm{Tr}\, U_x = e^{i\phi_{1x}} + e^{i\phi_{2x}} + e^{-i(\phi_{1x}+\phi_{2x})}$$

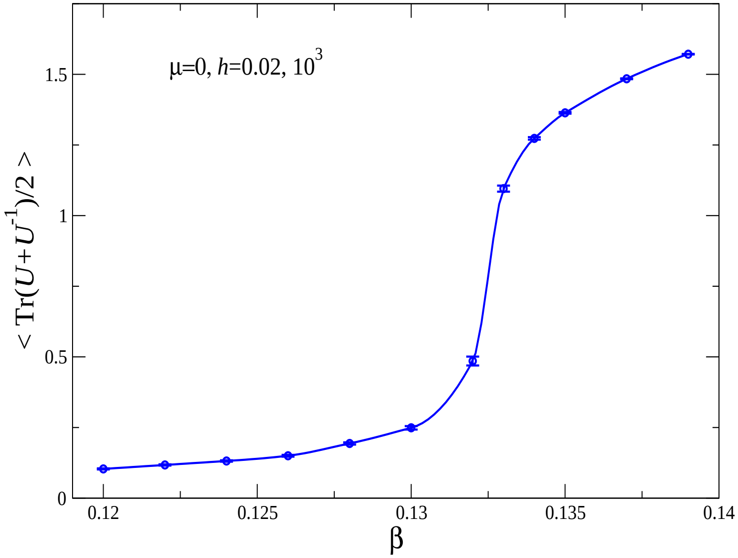
- Must include reduced Haar measure

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

- Effective action $S_{\mathrm{eff}} = S_B + S_F + S_H$
- Langevin dynamics then given by

$$\frac{\partial}{\partial\vartheta}\phi_{ax} = K_{ax} + \eta_{ax}, \qquad K_{ax} = -\frac{\partial S_{\mathrm{eff}}}{\partial\phi_{ax}}$$

Phase transition at $\mu = 0$



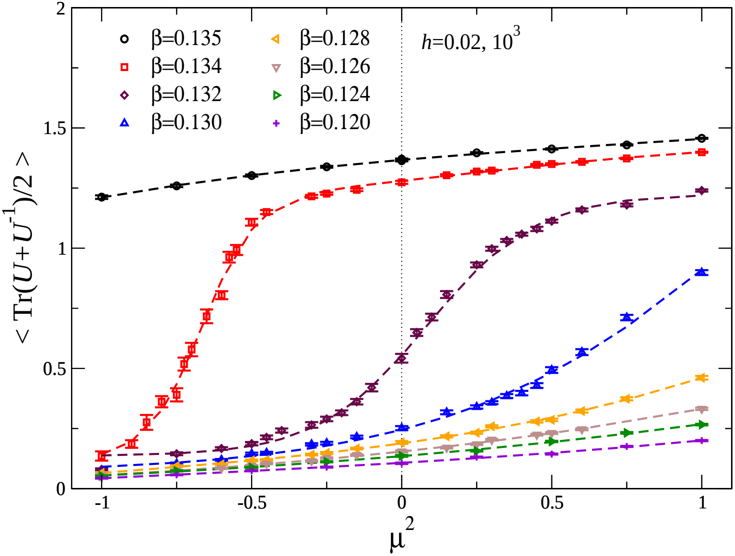
Imaginary chemical potential

- With imaginary chemical potential the action is real, no sign problem
- Complex Langevin results should be continuous across $\mu^2 = 0$ from the imaginary chemical potential results
- Non-analyticity is a sign of convergence to wrong limit
- XY model is an example of non-analyticity and incorrect convergence, where CL failed in part of the phase diagram

Aarts and FJ, 2010

- Choose observable even in μ, $\langle \mathrm{Tr}\,(U + U^{-1})\rangle/2$

Analyticity in μ^2



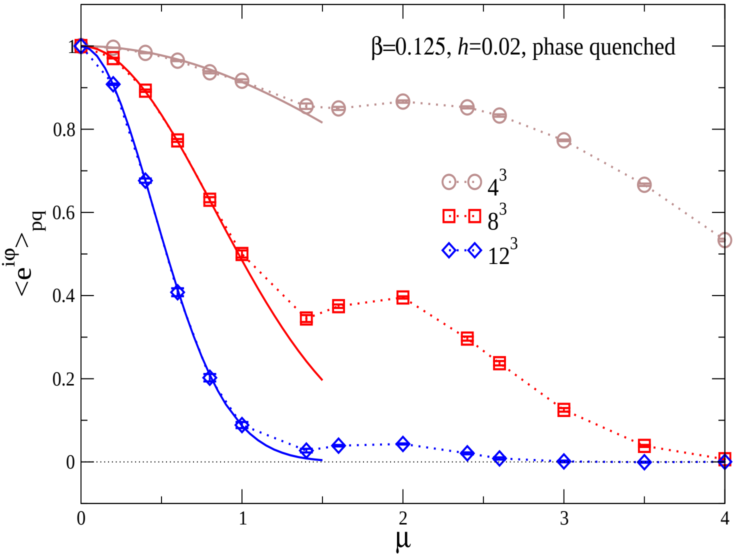
Taylor series expansion

- Can perform a Taylor series expansion in μ
- Simulations at $\mu = 0$ used to extrapolate to $\mu > 0$
- Provides test for correct results at $\mu \neq 0$ for small chemical potentials
- Free energies in full and phase quenched theories:

$$f(\mu) = f(0) - (c_1 + c_2 h) h\mu^2 + O(\mu^4)$$
$$f_{\mathrm{pq}}(\mu) = f(0) - c_1 h\mu^2 + O(\mu^4)$$

- With

$$c_1 = \frac{1}{\Omega} \sum_x \langle \mathrm{Tr}\, U_x \rangle_{\mu=0} = 0.1146(21),$$
$$c_2 = \frac{1}{2\Omega} \sum_{xy} \langle \mathrm{Tr}\,(U_x - U_x^\dagger) \mathrm{Tr}\,(U_y - U_y^\dagger) \rangle_{\mu=0} = -3.534(72)$$


β=0.125, h=0.02, phase quenched
4^3
8^3
12^3
$<e^{i\varphi}>_{pq}$
μ
0
0.2
0.4
0.6
0.8
1
0
1
2
3
4

Density and Silver Blaze problem

- Silver Blaze problem: $\mu \neq 0$ but observables μ-independent
- Requires precise cancellations in numerical simulations
- Density given by

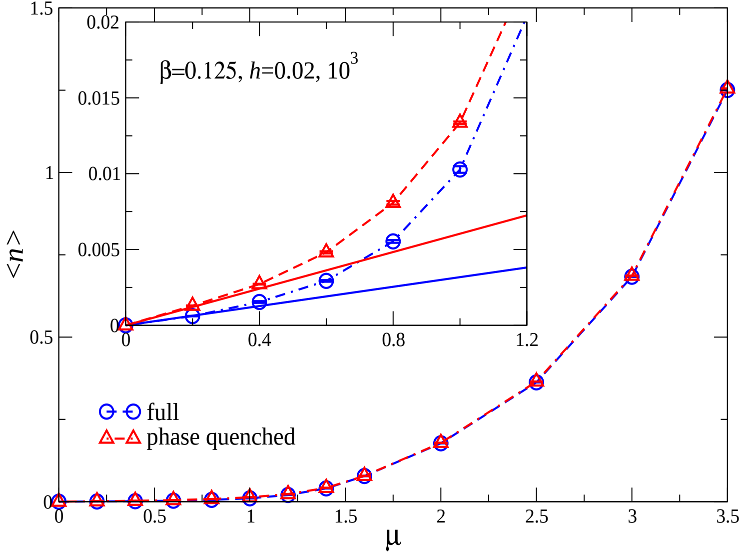
$$\langle n \rangle = \frac{1}{\Omega} \frac{\partial \ln Z}{\partial \mu} = \langle h e^{\mu} \mathrm{Tr}\, U_x - h e^{-\mu} \mathrm{Tr}\, U_x^{\dagger} \rangle$$

- When $\mu \neq 0$ there is a difference between $\langle \mathrm{Tr}\, U \rangle$ and $\langle \mathrm{Tr}\, U^{\dagger} \rangle$
- Silver Blaze effect requires μ-independence: $\langle \mathrm{Tr}\, U \rangle = \langle \mathrm{Tr}\, U^{\dagger} \rangle$
- Not possible to satisfy both requirements: no Silver Blaze here
- Phase quenched:

$$\langle n \rangle_{\mathrm{pq}} = h \sinh \mu \langle \mathrm{Tr}\, U_x + \mathrm{Tr}\, U_x^{\dagger} \rangle_{\mathrm{pq}}$$

- $\langle n \rangle_{\mathrm{pq}} \neq 0$ immediately once $\mu \neq 0$

Density Taylor expansion



Improved algorithm

- Need to extrapolate to vanishing stepsize $\epsilon \to 0$
- Standard algorithm (Euler integration) has $O(\epsilon)$ corrections
- Simple mid-point scheme with improved drift terms but noise unchanged does not improve corrections
- Must also modify noise terms
- An improved algorithm proposed for real Langevin dynamics

  Chien-Cheng Chang, 1987
- Reduces corrections to $O(\epsilon^2)$ for free theories and $O(\epsilon^{3/2})$ for coupled systems

Improved algorithm

- Add intermediate steps $\psi, \tilde{\psi}$ and modify noise terms

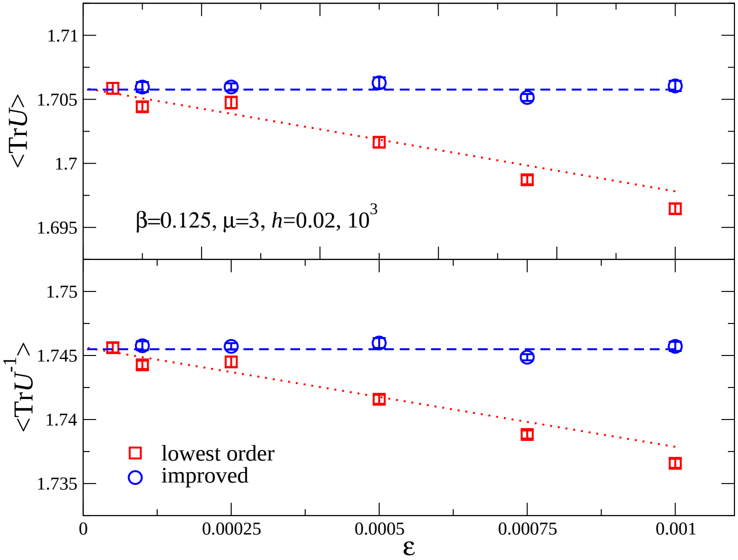
$$\psi_{ax}(n) = \phi_{ax}(n) + \frac{1}{2}\epsilon K[\phi_{ax}(n)] + k\sqrt{\epsilon}\tilde{\alpha}_{ax}(n),$$
$$\tilde{\psi}_{ax}(n) = \phi_{ax}(n) + \frac{1}{2}\epsilon K[\phi_{ax}(n)] + l\sqrt{\epsilon}\tilde{\alpha}_{ax}(n),$$
$$\phi_{ax}(n+1) = \phi_{ax}(n) + \epsilon\left(aK[\psi_{ax}(n)] + bK[\tilde{\psi}_{ax}(n)]\right) + \sqrt{\epsilon}\alpha_{ax}(n)$$

- Coefficients chosen to cancel $O(\epsilon)$ contributions:

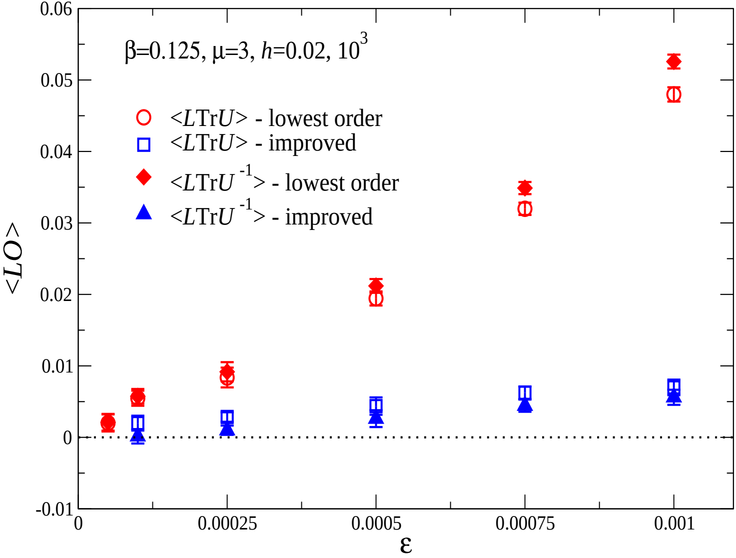
$$a = \frac{1}{3}, \quad b = \frac{2}{3}, \quad k = 0, \quad l = \frac{3}{2}$$

- Random variable $\tilde{\alpha}_{ax}(n) = \frac{1}{2}\alpha_{ax}(n) + \frac{\sqrt{3}}{6}\xi_{ax}(n)$
- Gaussian noise terms α, ξ

Stepsize corrections: observables



Stepsize corrections: criteria



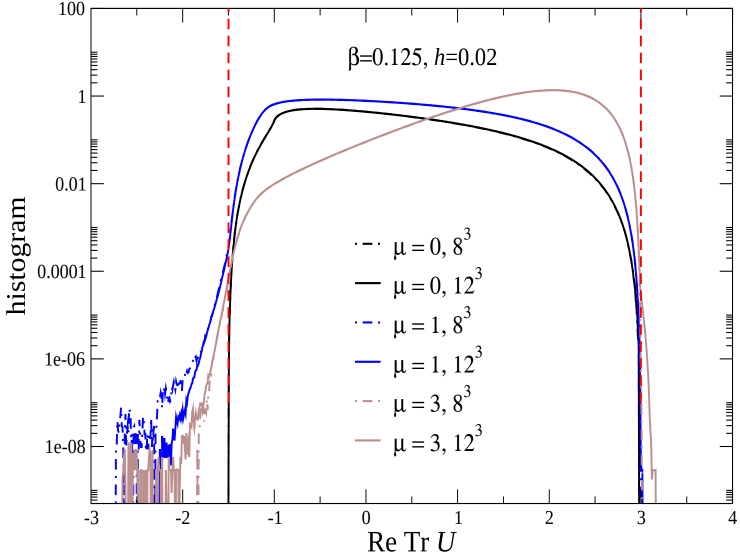
Criteria for correctness

- Clear linear stepsize correction with standard algorithm
- Stepsize corrections much smaller with improved algorithm
- Find that $\langle LO \rangle$ vanish in limit of $\epsilon \to 0$
- Note: condition must be satisfied even with real Langevin dynamics
- Condition that $\langle LO \rangle = 0$ therefore quantifies stepsize corrections

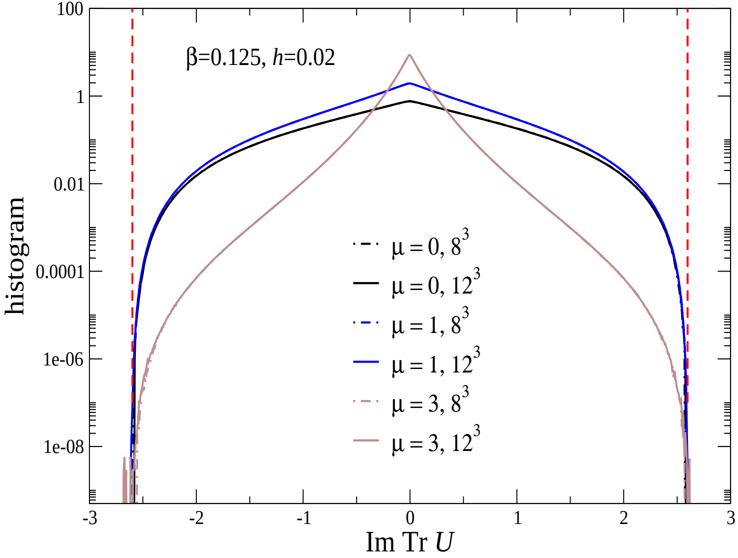
Distribution of observables

- Compute histogram of observables during Langevin evolution
- Gives a distribution of values sampled by the process
- Complexified space should be explored
- Need distribution sufficiently localised for criteria to be satisfied
- Look at distributions of $\mathrm{Re}\mathrm{Tr}\, U, \mathrm{Im}\mathrm{Tr}\, U$

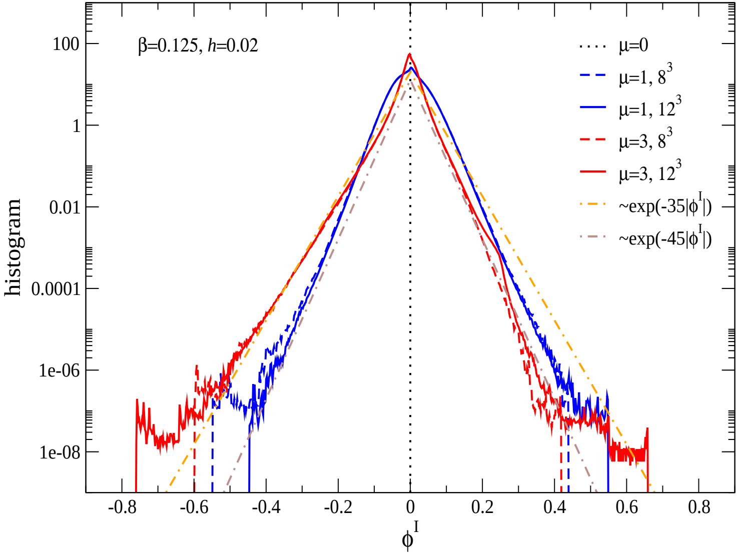
Distributions: Tr U



Distributions: Tr U



Distributions: ϕ^{I}



Decay of ϕ^{I}

- Decay of $P(\phi^{\mathrm{I}}) \sim e^{-a|\phi^{\mathrm{I}}|}$, with $a \sim 40$
- Rapid decay enough for correct convergence of $O = \mathrm{Tr}\, U$
- Problem for observables of high powers like $\mathrm{Tr}\,[U^k]$ for $k \gtrsim 40$
- Contributions are like $e^{-k\phi^{\mathrm{I}}} \cos(k\phi^{\mathrm{R}})$
- These should vanish due to oscillating sign?
- Compare with U(1) one-link model where $a \sim 2$ and complex Langevin failed Aarts, FJ, Seiler, Stamatescu, 2011

Complex neighbours

- Focus on single lattice site x

$$S = -\sum_x \mathrm{Tr}\, U_x \left(\beta \sum_\nu [\mathrm{Tr}\, U^\dagger_{x+\hat{\nu}} + \mathrm{Tr}\, U^\dagger_{x-\hat{\nu}}] + he^{\mu} \right) + \mathrm{Tr}\, U^\dagger_x \left(\beta \sum_\nu [\mathrm{Tr}\, U_{x+\hat{\nu}} + \mathrm{Tr}\, U_{x-\hat{\nu}}] + he^{-\mu} \right)$$

- Combine neighbours

$$u_x = \frac{1}{6} \sum_{\nu=1}^{3} \mathrm{Tr}\, U^\dagger_{x+\hat{\nu}} + \mathrm{Tr}\, U^\dagger_{x-\hat{\nu}}$$

- Action

$$S = -\sum_x (6\beta u_x + he^{\mu}) \mathrm{Tr}\, U_x + (6\beta u^*_x + he^{-\mu}) \mathrm{Tr}\, U^\dagger$$

Effective 1-link model

- Action

$$S = -\beta_1 \mathrm{Tr}\, U - \beta_2 \mathrm{Tr}\, U^\dagger$$

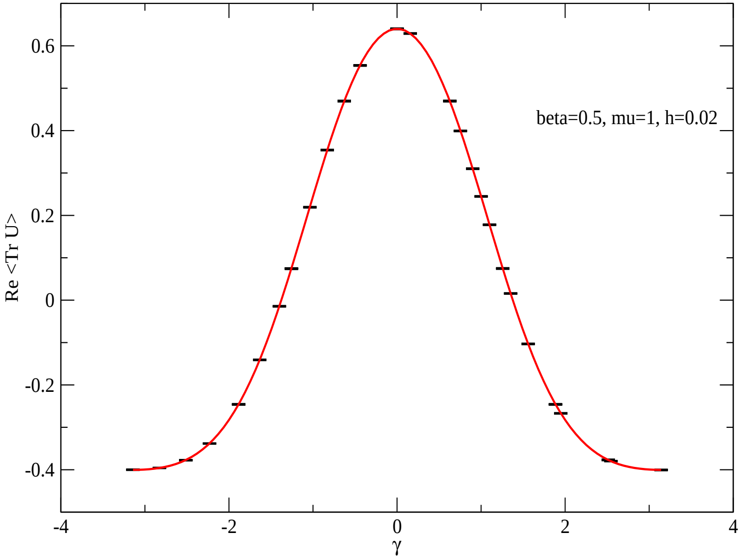
- Complex parameters

$$\beta_1 = \beta_{\mathrm{eff}}\, e^{i\gamma} + he^{\mu}, \qquad \beta_2 = \beta_{\mathrm{eff}}\, e^{-i\gamma} + he^{-\mu}$$

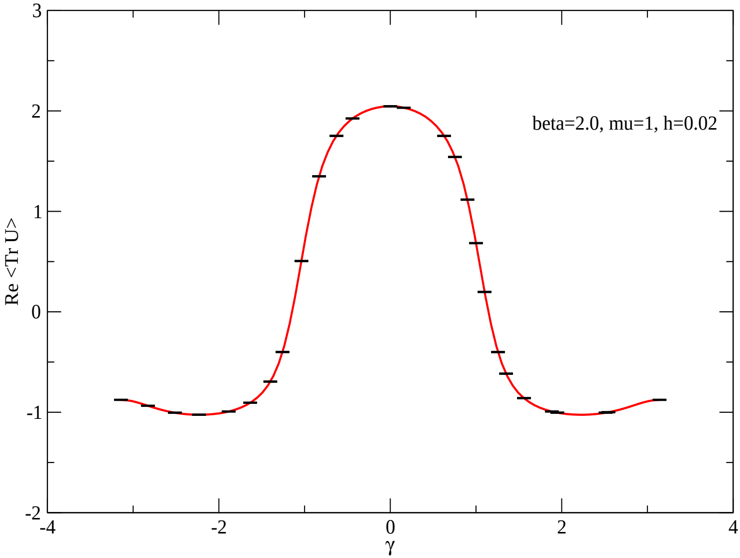
- Couplings related to full model $\beta_{\mathrm{eff}}\, e^{i\gamma} = 6\beta u$
- Write with angles, gain reduced Haar measure

$$S_H = -\log\left[\sin^2\left(\frac{\phi_1 - \phi_2}{2}\right)\sin^2\left(\frac{2\phi_1 + \phi_2}{2}\right)\sin^2\left(\frac{\phi_1 + 2\phi_2}{2}\right)\right]$$

Results



Results



Conclusions

- Complex Langevin dynamics is still a candidate for circumventing sign problem
- Criteria provide necessary conditions for correct results
- Improved algorithm eliminates leading order stepsize corrections
- Criteria also provide general method for quantifing stepsize corrections
- SU(3) spin model passes the tests for correct results on both sides of phase diagram
- Effective 1-link model works for all complex parameters
- No dependence on severeness of sign problem and performance of complex Langevin dynamics