Complex Langevin dynamics for gauge theories

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Outline

- into complex plane
- real/complex Langevin dynamics: theory
- stability, convergence, and all that

- SU(3) spin model
- analytical solution for distributions
- SU(N) and gauge cooling
- QCD with heavy quarks

GA, *Introductory lectures on lattice QCD at nonzero baryon number*, J. Phys. Conf. Ser. 706 022004 [arXiv:1512.05145 [hep-lat]].

Caveats

- incomplete overview
- focus on work with Seiler, Stamatescu, Sexty, . . .
- recent results not included
- incomplete references

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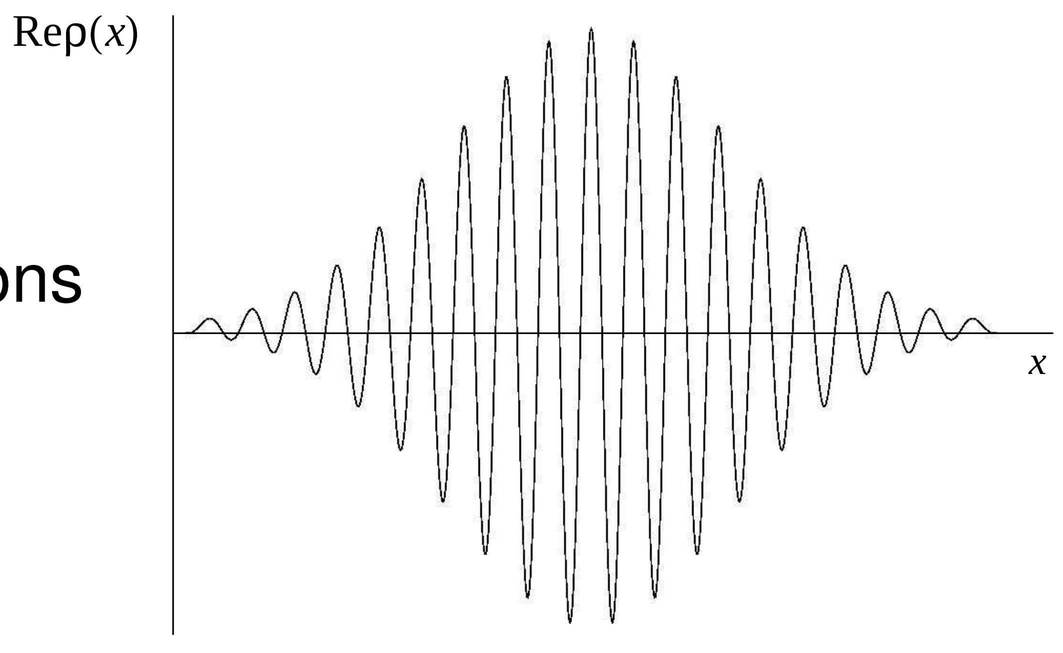
machine learning: cat or dog/chihuahua or muffin

Overlap problem

$$Z = \int D\phi \, e^{-S} \qquad\qquad S \in \mathbb{C}$$

- configurations differ in an essential way from those obtained at with $|e^{-S}|$
- cancelation between configurations with ‘positive’ and ‘negative’ weight

dominant configurations
in the path integral?



Complex integrals

- consider simple integral

$$Z(a,b) = \int_{-\infty}^{\infty} dx\, e^{-S(x)} \qquad\qquad S(x) = ax^2 + ibx$$

- complete the square/saddle point approximation:

  into complex plane

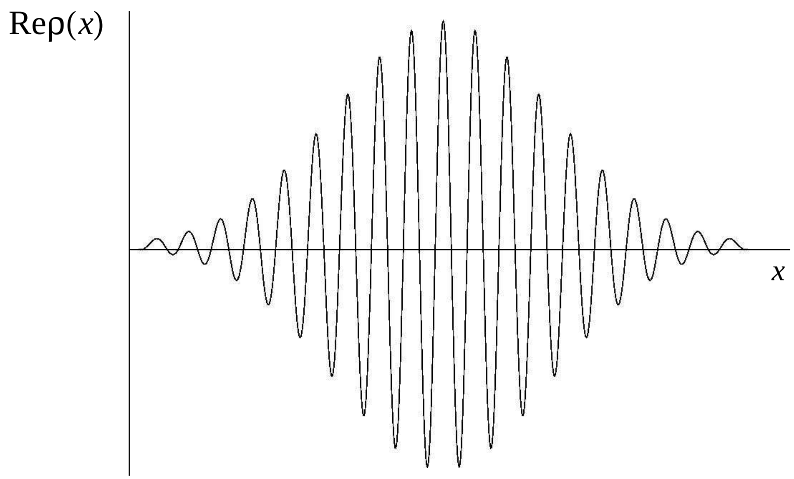
- lesson: don't be real(istic), be more imaginative

radically different approach:

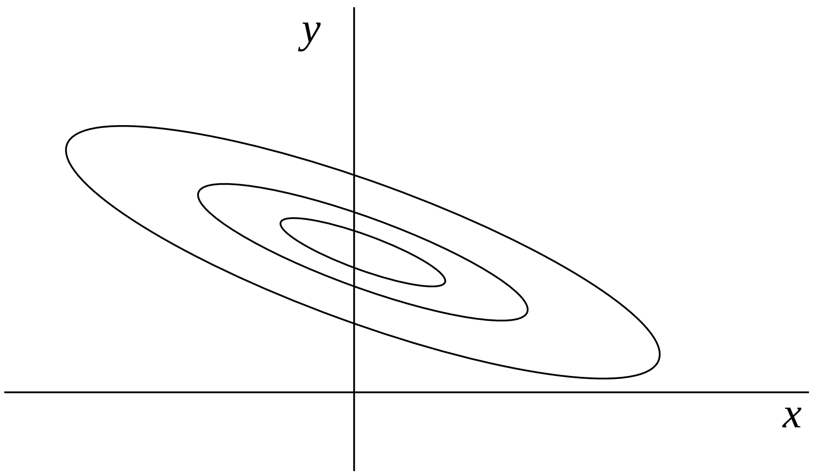
- complexify all degrees of freedom $x \to z = x + iy$
- enlarged complexified space
- new directions to explore

Complexified field space

dominant configurations in the path integral?



$\Rightarrow$



real and positive distribution $P(x, y)$: how to obtain it?

$\Rightarrow$ solution of stochastic process

$$\boxed{\text{complex Langevin dynamics}}$$

Parisi 83, Klauder 83

Real Langevin dynamics

partition function $Z = \int dx\, e^{-S(x)}$ $\qquad S(x) \in \mathbb{R}$

- Langevin equation

$$\dot{x} = -\partial_x S(x) + \eta, \qquad \langle \eta(t)\eta(t')\rangle = 2\delta(t-t')$$

- associated distribution $\rho(x,t)$

$$\langle O(x(t)\rangle_\eta = \int dx\, \rho(x,t) O(x)$$

- Langevin eq for $x(t)$ $\quad \Leftrightarrow \quad$ Fokker-Planck eq for $\rho(x,t)$

$$\dot{\rho}(x,t) = \partial_x \left(\partial_x + S'(x)\right) \rho(x,t)$$

- stationary solution: $\quad \rho(x) \sim e^{-S(x)}$

Fokker-Planck equation

- stationary solution typically reached exponentially fast

$$\dot{\rho}(x,t) = \partial_x \left(\partial_x + S'(x)\right) \rho(x,t)$$

- write $\quad \rho(x,t) = \psi(x,t)e^{-\frac{1}{2}S(x)}$

$$\dot{\psi}(x,t) = -H_{\rm FP}\psi(x,t)$$

- Fokker-Planck hamiltonian:

$$H_{\rm FP} = Q^\dagger Q = \left[-\partial_x + \frac{1}{2}S'(x)\right]\left[\partial_x + \frac{1}{2}S'(x)\right] \geq 0$$

$$Q\psi(x) = 0 \qquad \Leftrightarrow \qquad \psi(x) \sim e^{-\frac{1}{2}S(x)}$$

$$\psi(x,t) = c_0 e^{-\frac{1}{2}S(x)} + \sum_{\lambda>0} c_\lambda e^{-\lambda t} \to c_0 e^{-\frac{1}{2}S(x)}$$

Complex Langevin dynamics

partition function $Z = \int dx\, e^{-S(x)}$ $\qquad S(x) \in \mathbb{C}$

- complex Langevin equation: complexify $x \to z = x + iy$

$$\begin{aligned} \dot{x} &= -\mathrm{Re}\, \partial_z S(z) + \eta & \qquad \langle \eta(t)\eta(t')\rangle &= 2\delta(t-t') \\ \dot{y} &= -\mathrm{Im}\, \partial_z S(z) & S(z) &= S(x+iy) \end{aligned}$$

- associated distribution $P(x, y; t)$

$$\langle O(x+iy)(t)\rangle = \int dxdy\, P(x,y;t) O(x+iy)$$

- Langevin eq for $x(t), y(t)$ $\quad \Leftrightarrow \quad$ FP eq for $P(x, y; t)$

$$\dot{P}(x,y;t) = \left[\partial_x \left(\partial_x + \mathrm{Re}\ \partial_z S\right) + \partial_y \mathrm{Im}\ \partial_z S\right] P(x,y;t)$$

- generic solutions? semi-positive FP hamiltonian?

Equilibrium distributions

complex weight $\rho(x)$ real weight $P(x, y)$

- main premise:

$$\int dx\, \rho(x) O(x) = \int dxdy\, P(x, y) O(x + iy)$$

- if equilibrium distribution $P(x, y)$ is known analytically: shift variables

$$\int dxdy\, P(x, y) O(x + iy) = \int dx\, O(x) \int dy\, P(x - iy, y)$$

$$\Rightarrow \rho(x) = \int dy\, P(x - iy, y)$$

- correct when $P(x, y)$ is known analytically
- hard to verify in numerical studies!

Field theory

- path integral $Z = \int D\phi \, e^{-S}$
- Langevin dynamics in “fifth” time direction

$$\frac{\partial \phi(x,t)}{\partial t} = -\frac{\delta S[\phi]}{\delta \phi(x,t)} + \eta(x,t)$$

- Gaussian noise

$$\langle \eta(x,t) \rangle = 0 \qquad \langle \eta(x,t)\eta(x',t') \rangle = 2\delta(x-x')\delta(t-t')$$

- compute expectation values $\langle \phi(x,t)\phi(x',t) \rangle$, etc
- study converge as $t \to \infty$

Parisi & Wu 81, Parisi, Klauder 83
Damgaard & Hüffel 87

Some achievements

complex Langevin dynamics *can*

- handle severe sign problems . . .
  . . . in thermodynamic limit
- describe onset at expected critical chemical potential
  i.e. not at phase-quenched value (Silver Blaze problem)
- describe phase transitions
- be implemented for gauge theories

however, success is not guaranteed

Troubled past

1. numerical problems: runaways, instabilities

   $\Rightarrow$ adaptive stepsize

   no instabilities observed, works for SU(3) gauge theory

   GA, James, Seiler & Stamatescu, 0912.0617

   a la Ambjorn et al 86

2. theoretical status unclear

   $\Rightarrow$ detailed analyis, identified necessary conditions

   GA, FJ, ES & IOS, 0912.3360, 1101.3270

3. convergence to wrong limit

   $\Rightarrow$ better understood but not yet resolved

   GA, ES, DS & IOS, 1701.02322

Analytical understanding

consider expectation values and Fokker-Planck equations

one degree of freedom x, complex action $S(x)$, $\rho(x) \sim e^{-S(x)}$

- wanted: $$\langle O\rangle_{\rho(t)} = \int dx\ \rho(x,t)O(x)$$
$$\partial_t\rho(x,t) = \partial_x\left(\partial_x + S'(x)\right)\rho(x,t)$$

- solved with CLE:
$$\langle O\rangle_{P(t)} = \int dxdy\ P(x,y;t)O(x+iy)$$
$$\partial_t P(x,y;t) = \left[\partial_x\left(\partial_x - K_x\right) - \partial_y K_y\right]P(x,y;t)$$

  with $K_x = -\mathrm{Re}S'$, $K_y = -\mathrm{Im}S'$

- question: $\langle O\rangle_{P(t)} = \langle O\rangle_{\rho(t)}$ if $P(x,y;0) = \rho(x;0)\delta(y)$?

Analytical understanding

question: $\langle O\rangle_{P(t)} = \langle O\rangle_{\rho(t)}$ as $t \to \infty$?

answer: yes, use Cauchy-Riemann equations
and satisfy some conditions:

- distribution $P(x, y)$ should drop off fast enough in y direction
- partial integration without boundary terms possible
- actually $O(x + iy)P(x, y)$ for large enough set $O(x)$

$\Rightarrow$ distribution should be sufficiently localized

- can be tested numerically via criteria for correctness

$$\langle LO(x + iy)\rangle = 0$$

with L Langevin operator 0912.3360, 1101.3270

SU(3) spin model

apply these ideas to 3D SU(3) spin model

GA & James, 1112.4655

- earlier solved with complex Langevin Karsch & Wyld 85

  Bilic, Gausterer & Sanielevici 88
- however, no detailed tests performed

$\Rightarrow$ test reliability of complex Langevin using developed tools

- analyticity in μ^2:
  - from imaginary to real μ
  - Taylor series
- criteria for correctness
- comparison with flux formulation Gattringer & Mercado 12

SU(3) spin model

3-dimensional SU(3) spin model: $S = S_B + S_F$

$$S_B = -\beta \sum_{<xy>} \left[P_x P_y^* + P_x^* P_y \right]$$

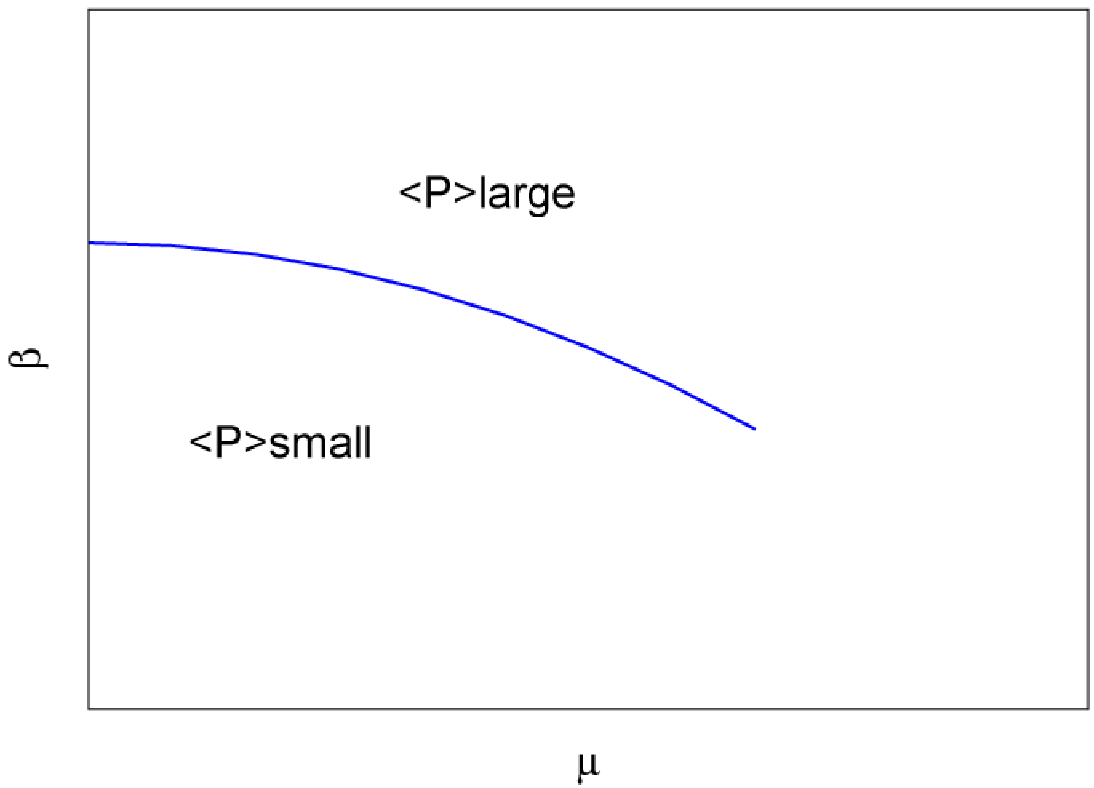
$$S_F = -h \sum_x \left[e^{\mu} P_x + e^{-\mu} P_x^* \right]$$

- SU(3) matrices: $P_x = \mathrm{Tr}\, U_x$
- gauge action: nearest neighbour Polyakov loops
- (static) quarks represented by Polyakov loops
- complex action $S^*(\mu) = S(-\mu^*)$

effective model for QCD with static quarks, centre symmetry

SU(3) spin model

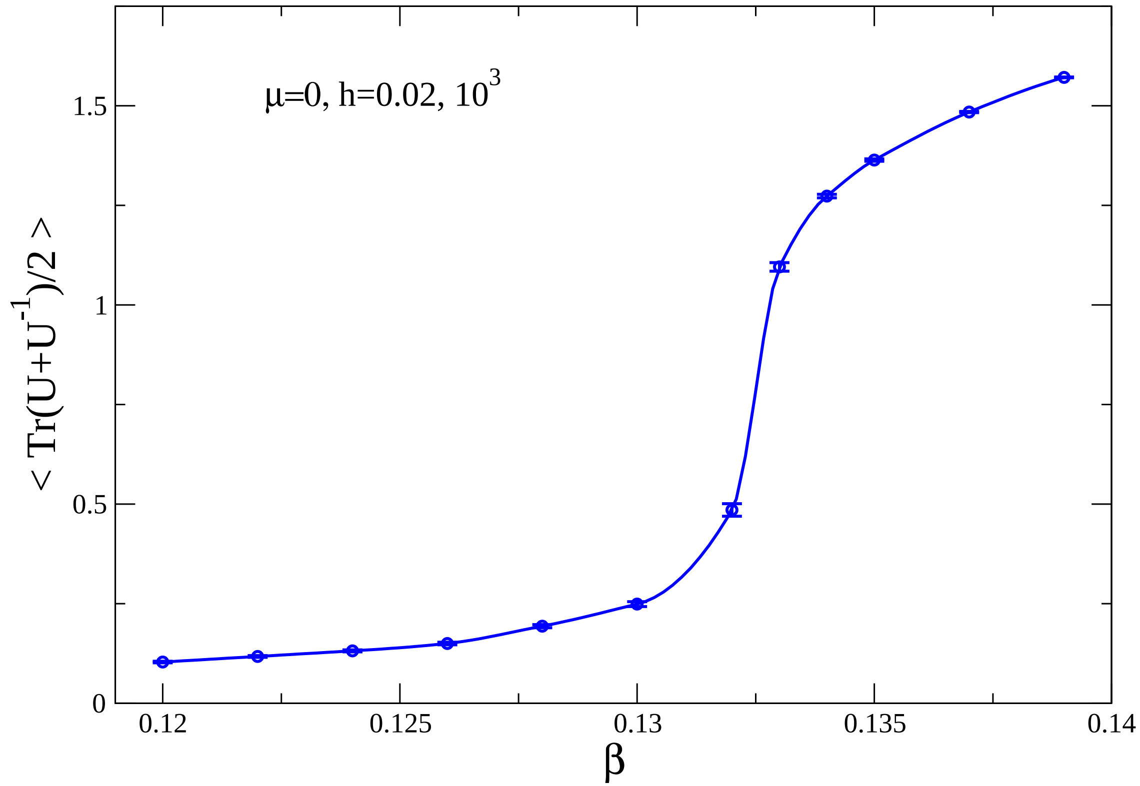
- phase structure



- effective model for QCD with static quarks

SU(3) spin model

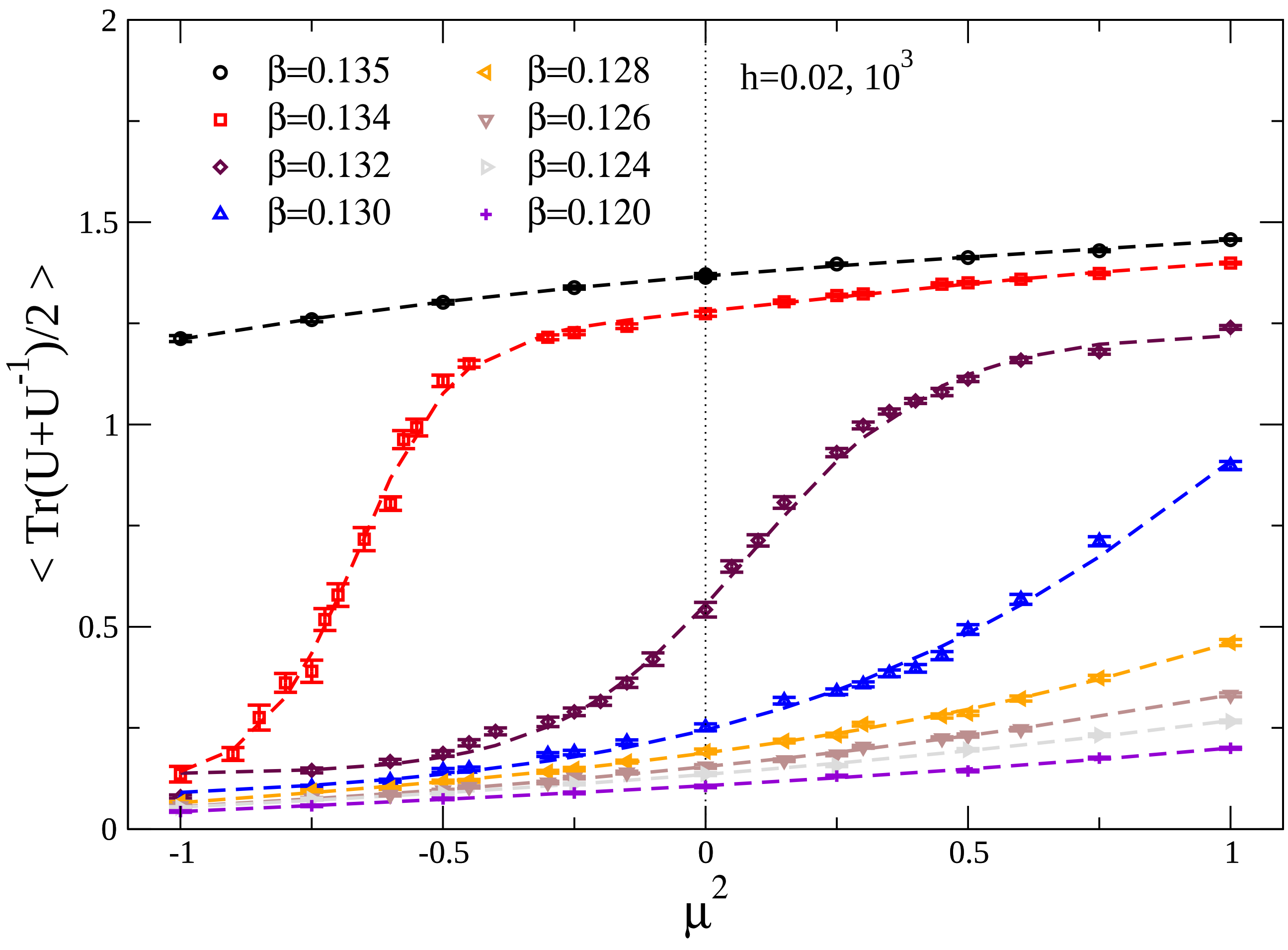
- phase structure at $\mu = 0$: $\langle P + P^{*} \rangle / 2$



SU(3) spin model

real and imaginary potential:

first-order transition in $\beta - \mu^2$ plane, $\langle P + P^* \rangle/2$



negative μ^2: real Langevin — positive μ^2: complex Langevin

SU(3) spin model

Taylor expansion (lowest order)

- free energy density

$$f(\mu) = f(0) - (c_1 + c_2 h)\, h\mu^2 + \mathcal{O}(\mu^4)$$

- density $\qquad \langle n \rangle = 2\,(c_1 + c_2 h)\, h\mu + \mathcal{O}(\mu^3)$
- Polyakov loops

$$\langle P \rangle = c_1 + c_2 h\mu + \mathcal{O}(\mu^2) \qquad \langle P^* \rangle = c_1 - c_2 h\mu + \mathcal{O}(\mu^2)$$

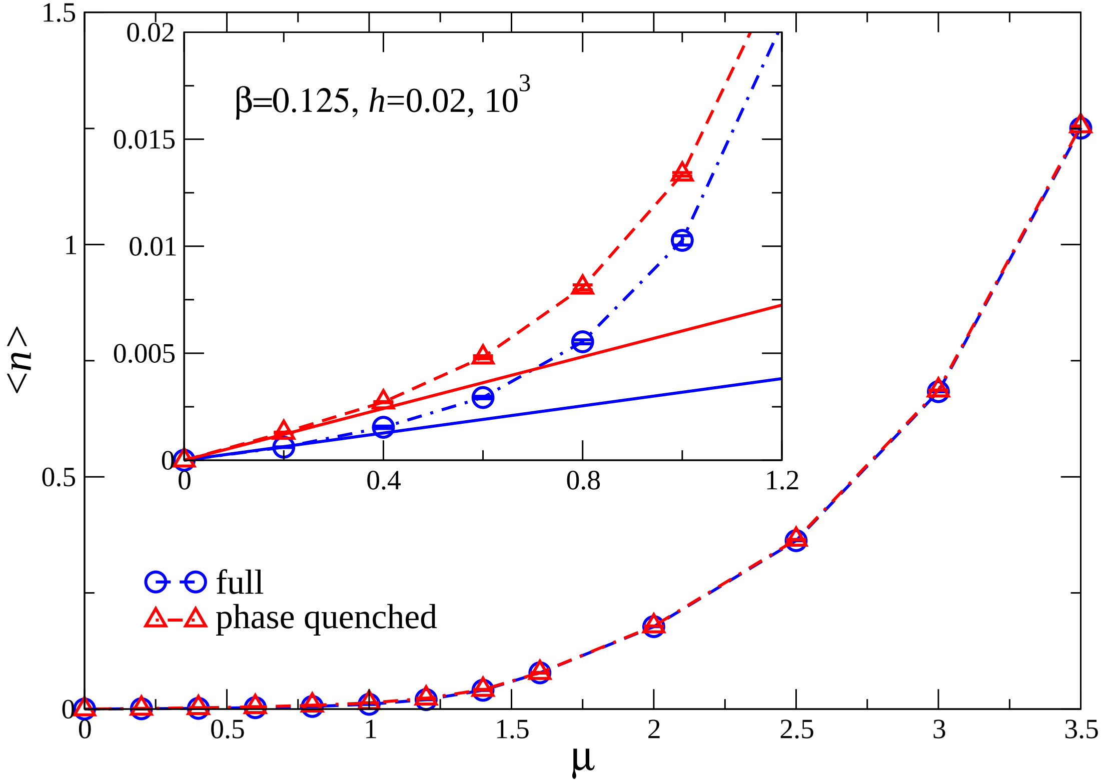
in terms of

$$c_1 = \frac{1}{\Omega} \sum_x \langle P_x \rangle_{\mu=0} \qquad c_2 = \frac{1}{2\Omega} \sum_{xy} \left\langle (P_x - P_x^*) \left(P_y - P_y^* \right) \right\rangle_{\mu=0}$$

c_2 is absent in phase-quenched theory

SU(3) spin model

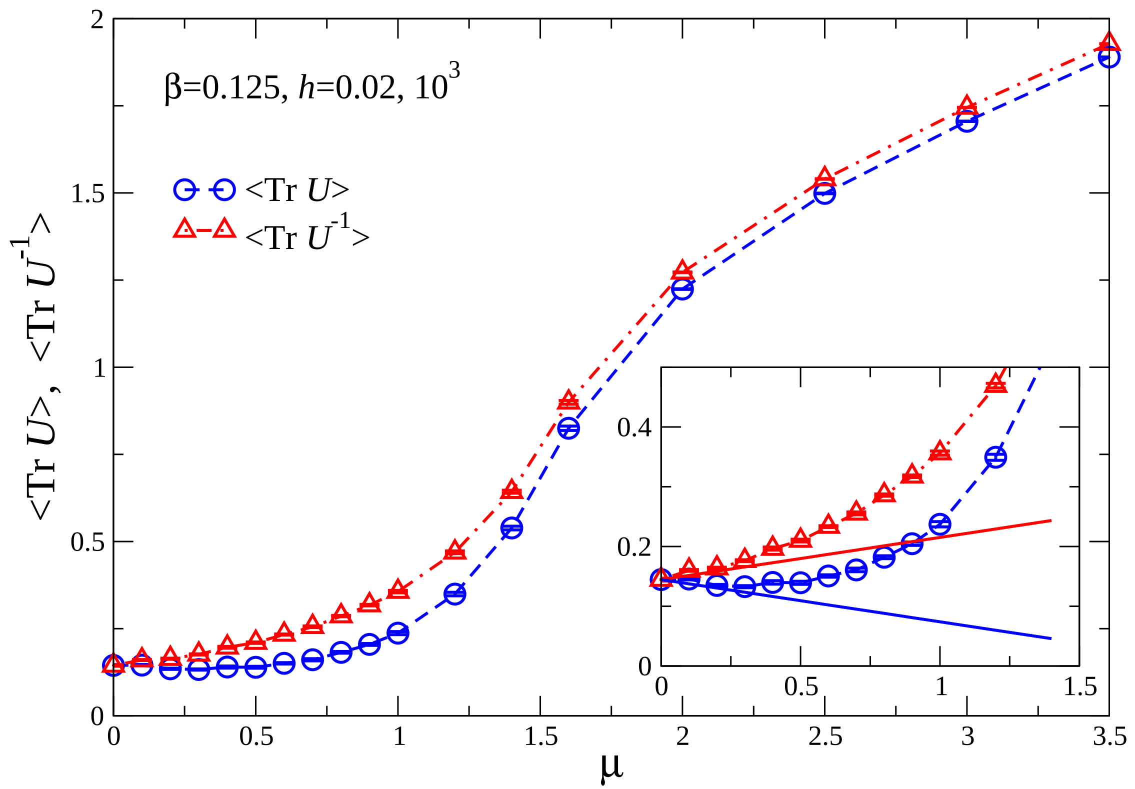
- start in 'confining' phase and increase μ
- density $\langle n\rangle = \langle he^{\mu}P_x - he^{-\mu}P_x^*\rangle$: no Silver Blaze region



- inset: lines from first-order Taylor expansion

SU(3) spin model

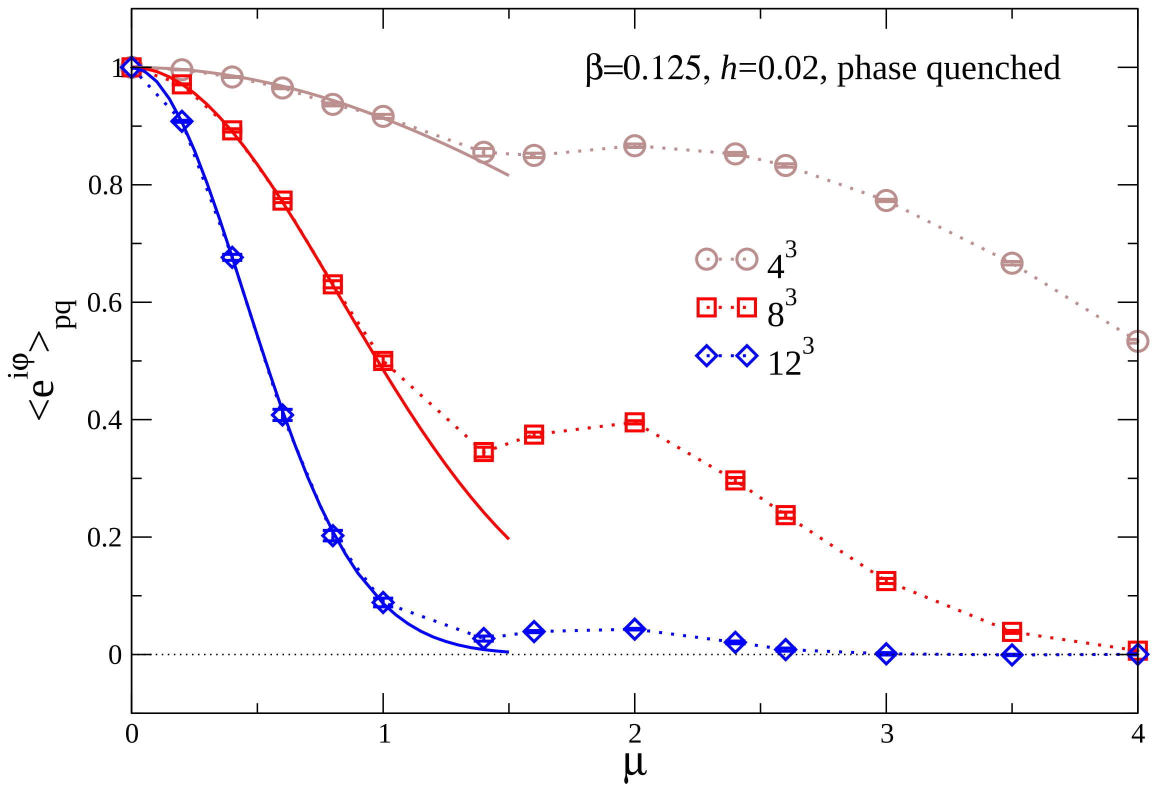
- start in 'confining' phase and increase μ
- splitting between $\langle P\rangle$ and $\langle P^*\rangle$: no Silver Blaze region



- inset: lines from first-order Taylor expansion

SU(3) spin model

- severeness of sign problem: $\langle e^{-i\mathrm{Im}S}\rangle_{\mathrm{pq}} = e^{-\Omega\Delta f}$



$$\Delta f \equiv f - f_{\mathrm{pq}} = -c_2 h^2 \mu^2 + \mathcal{O}(\mu^4) \qquad\qquad (c_2 < 0)$$

SU(3) spin model

- lowest-order discretization: $\phi_{n+1} = \phi_n + \epsilon K(\phi_n) + \sqrt{\epsilon}\eta_n$
- linear stepsize dependence: need extrapolation

higher order: Chien-Cheng Chang 87

$$\psi_n = \phi_n + \frac{1}{2}\epsilon K(\phi_n)$$

$$\tilde{\psi}_n = \phi_n + \frac{1}{2}\epsilon K(\phi_n) + \frac{3}{2}\sqrt{\epsilon}\,\tilde{\alpha}_n$$

$$\phi_{n+1} = \phi_n + \frac{1}{3}\epsilon\left[K(\psi_n) + 2K(\tilde{\psi}_n)\right] + \sqrt{\epsilon}\,\alpha_n$$

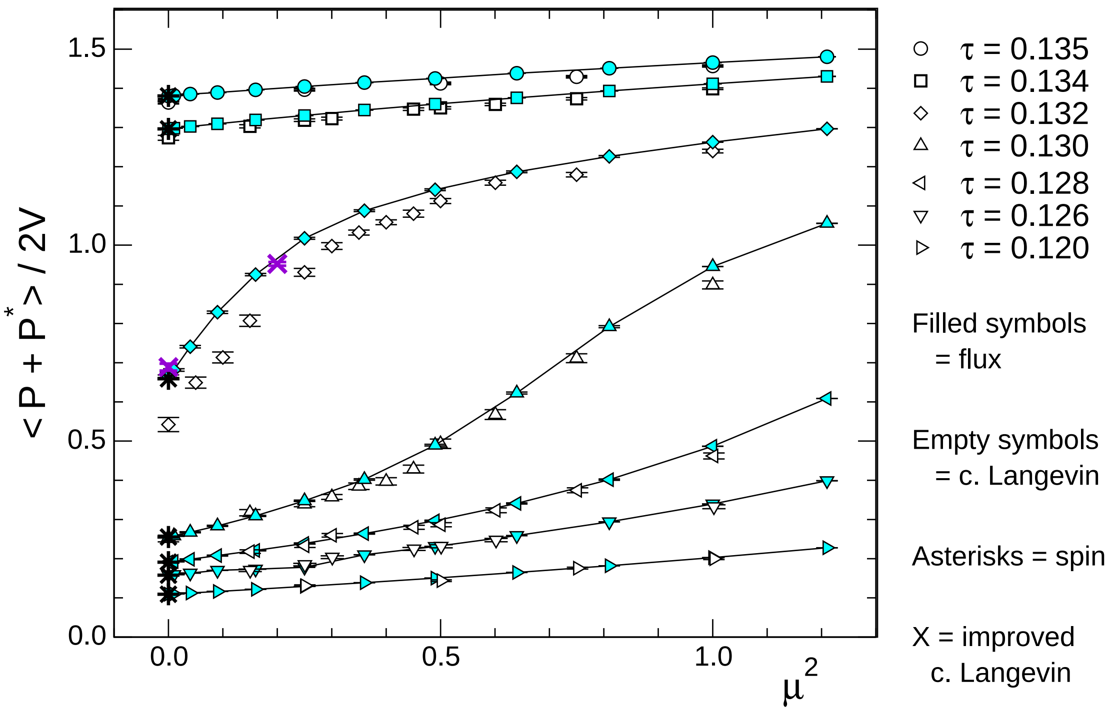
noise $\tilde{\alpha}_n = \frac{1}{2}\alpha_n + \frac{\sqrt{3}}{6}\xi_n \qquad \langle\alpha_n\alpha_{n'}\rangle = \langle\xi_n\xi_{n'}\rangle = 2\delta_{nn'}$

- very little stepsize dependence remaining in observables

SU(3) spin model

comparison with result obtained using flux representation

Gattringer & Mercado 12



- CL: finite stepsize errors in lowest-order algorithm
- improved algorithm removes discrepancy in critical region

Distributions

crucial role played by distribution $P(x, y)$

- does it exist?

  usually yes, constructed by brute force by solving the CL process

  direct solution of FP equation extremely hard

  `GA, ES & IOS 09, Duncan & Niedermaier 12, GA, PG & ES 13`

- what are its properties?

  localization in $x - y$ space, fast/slow decay at large $|y|$

  essential for mathematical justification of approach

  `GA, ES, IOS (& FJ) 09, 11`

- smooth connection with original distribution when the weight is real?

study with histograms, scatter plots, flow, FPE, $\ldots$

$\Rightarrow$ implications for gauge theories

Quartic model

$$Z = \int_{-\infty}^{\infty} dx\, e^{-S} \qquad\qquad S(x) = \frac{\sigma}{2}x^2 + \frac{\lambda}{4}x^4$$

complex mass parameter $\sigma = A + iB$, $\lambda \in \mathbb{R}$

often used toy model Ambjorn & Yang 85, Klauder & Petersen 85, Okamoto et al 89, Duncan & Niedermaier 12

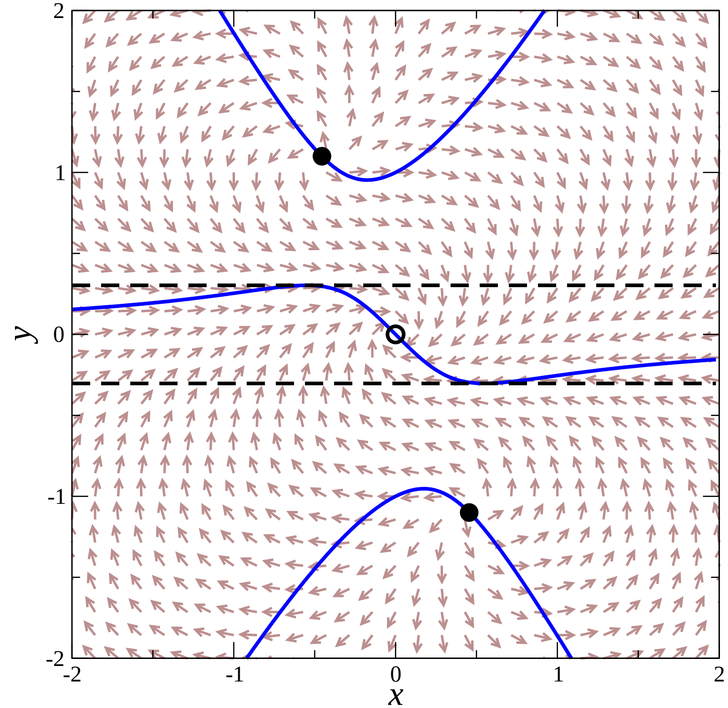
essentially analytical proof*: GA, Giudice & ES, 1306.3075

- CL gives correct result for all observables $\langle x^n \rangle$ provided that $A > 0$ and $A^2 > B^2/3$
- based on properties of the distribution $P(x, y)$
- follows from classical flow or directly from FPE

* 0912.3360, 1101.3270

Quartic model

classical flow
$(A = B = 1)$



- determine where drift $K_{\mathrm{I}} = -\mathrm{Im}\partial_z S(z)$ vanishes (blue lines)
- at the extrema: impenetrable barrier (for real noise)
- distribution localised between dashed lines

Quartic model

from Fokker-Planck equation:

- FPE can be written as $\dot{P} = \nabla \cdot \vec{J}$
- vanishing charge, with $\partial_y Q(y) = 0$,

$$Q(y) = \int dx\, J_y(x,y) = \int dx\, K_{\rm I}(x,y)P(x,y) = 0$$

since $P(x,y) \geq 0$:

- when $K_{\rm I}$ has definite sign, $P(x,y)$ has to vanish

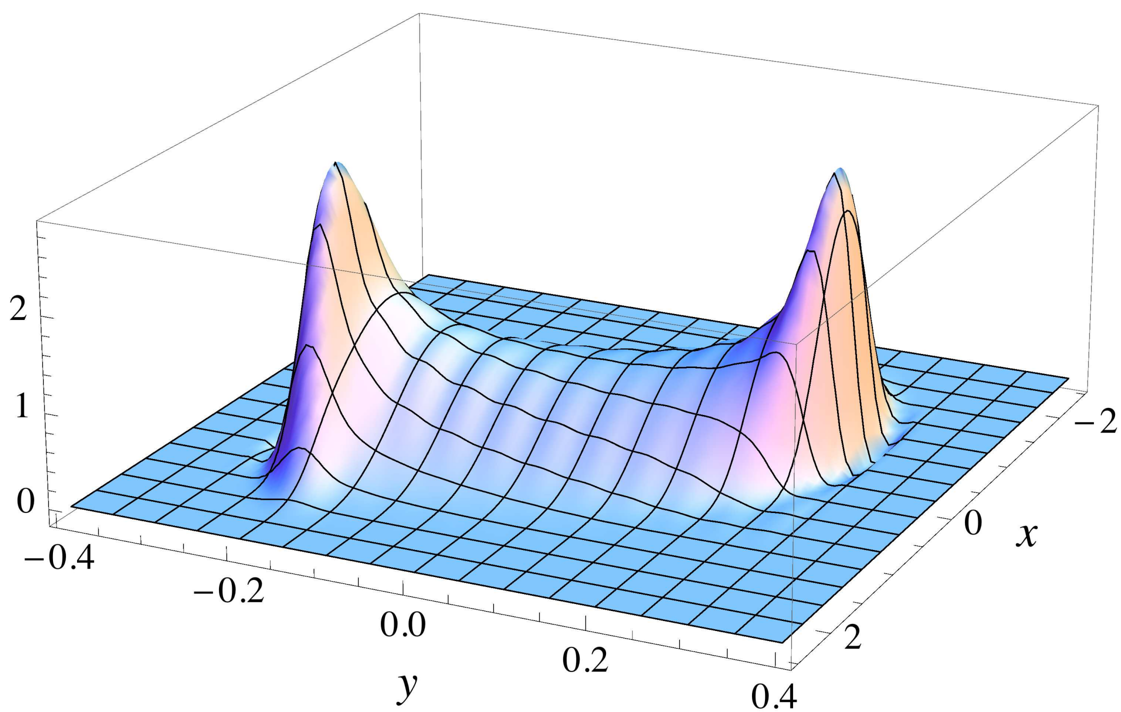
stripes: $$y_-^2 < y^2 < y_+^2$$

with

$$y_\pm^2 = \frac{1}{2\lambda}\left(A \pm \sqrt{A^2 - B^2/3}\right)$$

Quartic model

- numerical solution of FPE for $P(x, y)$
  following Duncan & Niedermaier 12
- distribution is localised in a strip around real axis
- $|y| < y_-$ with $y_- = 0.3029$ for $A = B = 1$



GA, Giudice & ES, 1306.3075

Localised distributions

if

- the action is holomorphic (no log dets!)

and

- the distribution is localised, i.e.

  $P(x,y) = 0$ for $|y| > y_{\max}$ [or $P(x,y) \to 0$ fast enough]

then

- the correct result is obtained

extend this to gauge theories ...

Gauge theories

SU(N) gauge theory: complexification to SL($N, \mathbb{C}$)

- links $U \in$ SU(N): CL update

$$U(n+1) = R(n)\,U(n) \qquad\qquad R = \exp\left[i\lambda_a\left(\epsilon K_a + \sqrt{\epsilon}\eta_a\right)\right]$$

Gell-mann matrices λ_a ($a = 1, \ldots N^2 - 1$)

- drift: $K_a = -D_a(S_B + S_F) \qquad S_F = -\ln\det M$

Gauge theories

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Gell-mann matrices λ_a ($a = 1, \ldots N^2 - 1$)

- drift: $\quad K_a = -D_a(S_B + S_F) \qquad S_F = -\ln\det M$

- complex action: $K^\dagger \neq K \Leftrightarrow U \in$ SL($N,\mathbb{C}$)

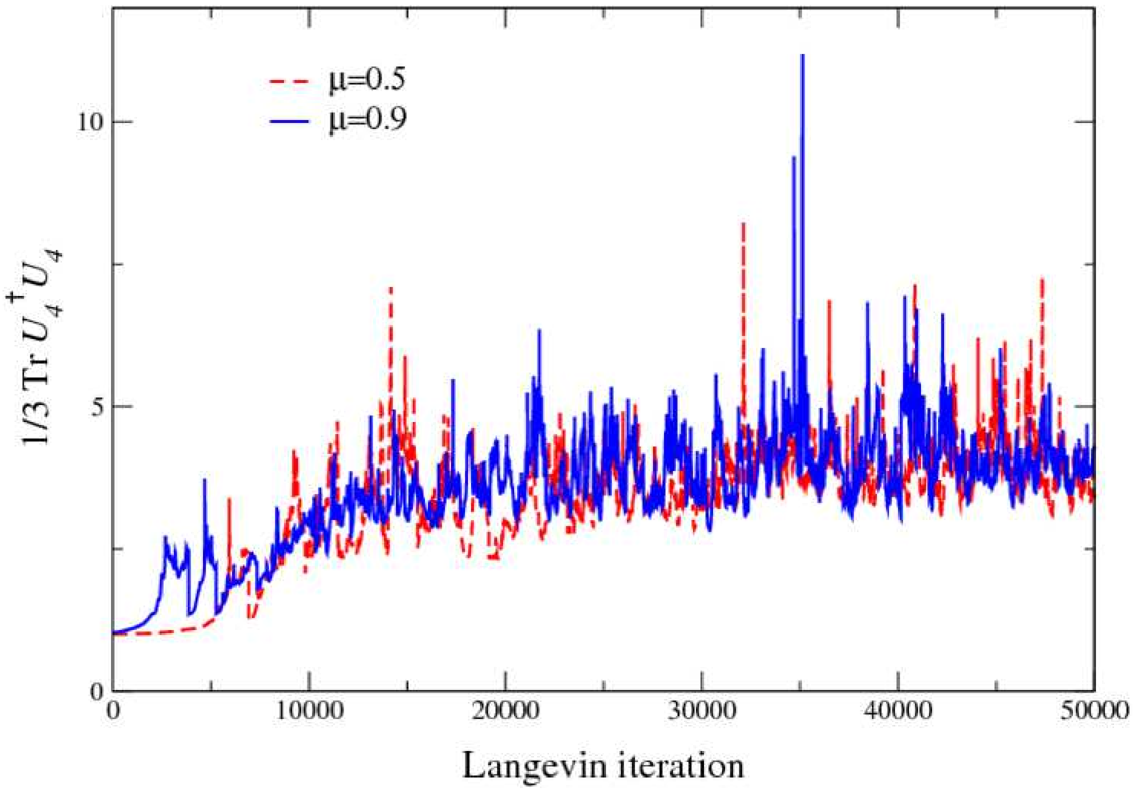
- deviation from SU(N): unitarity norms

$$\frac{1}{N}\mathrm{Tr}\,\left(UU^\dagger - 1\!\!1\right) \geq 0 \qquad\qquad \frac{1}{N}\mathrm{Tr}\,\left(UU^\dagger - 1\!\!1\right)^2 \geq 0$$

Gauge theories

deviation from SU(3): unitarity norm GA & IOS, 0807.1597

$$\frac{1}{3}\mathrm{Tr}\, UU^\dagger \geq 1$$



heavy dense QCD, 4^4 lattice with $\beta = 5.6$, $\kappa = 0.12$, $N_f = 3$

Gauge theories

controlled evolution: stay close to SU(N) submanifold when

- small chemical potential μ
- small non-unitary initial conditions
- in presence of roundoff errors

Gauge theories

controlled evolution: stay close to SU(N) submanifold when

- small chemical potential μ
- small non-unitary initial conditions
- in presence of roundoff errors

in practice this is not the case

$\Rightarrow$ unitary submanifold is unstable!

- process will not stay close to SU(N)
- wrong results in practice, e.g. jumps when μ^2 crosses 0
- also seen in abelian XY model

Unstable gauge theories

what is the origin? can this be fixed?

- gauge freedom: link at site k

$$U_k \to \Omega_k U_k \Omega_{k+1}^{-1} \qquad\qquad \Omega_k = e^{i\omega_a^k \lambda_a}$$

in SU(N): $\omega_a^k \in \mathbb{R}$ $\Rightarrow$ in SL($N, \mathbb{C}$): $\omega_a^k \in \mathbb{C}$

- choose ω_a^k purely imaginary, orthogonal to SU(N) direction

control unitarity norm $\frac{1}{N}\mathrm{Tr}\left(UU^\dagger - \mathbb{1}\right) \geq 0$

gauge cooling

ES, DS & IOS, 1211.3709

see also GA, LB, ES, DS & IOS, 1303.6425

Gauge cooling

cooling update at site k $\qquad \Omega_k = e^{-\alpha f_a^k \lambda_a} \qquad \alpha > 0$

$$U_k \to \Omega_k U_k \qquad U_{k-1} \to U_{k-1}\Omega_k^{-1}$$

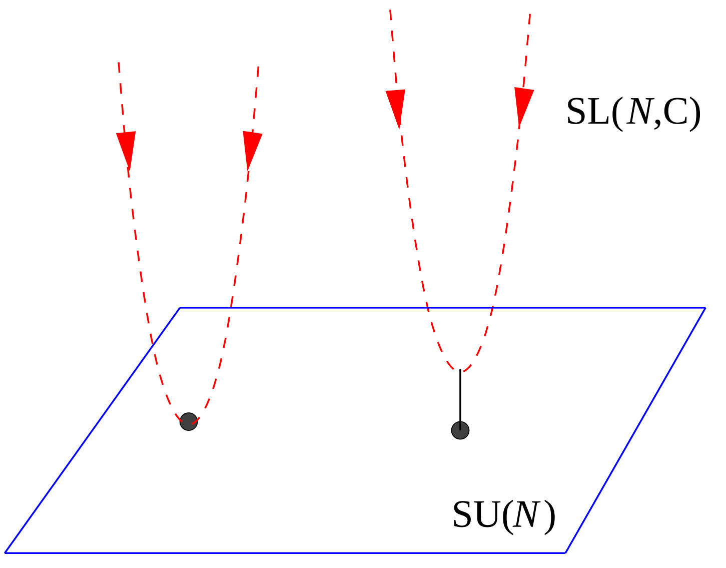
unitarity norm: distance $\qquad \mathrm{d} = \sum_k \frac{1}{N}\mathrm{Tr}\left(U_k U_k^\dagger - \mathbb{1}\right)$

after one update, $\mathrm{d} \to \mathrm{d}'$

linearise

$$\mathrm{d}' - \mathrm{d} = -\frac{\alpha}{N}(f_a^k)^2 + \mathcal{O}(\alpha^2) \le 0$$

reduce distance from SU(N)



Gauge cooling

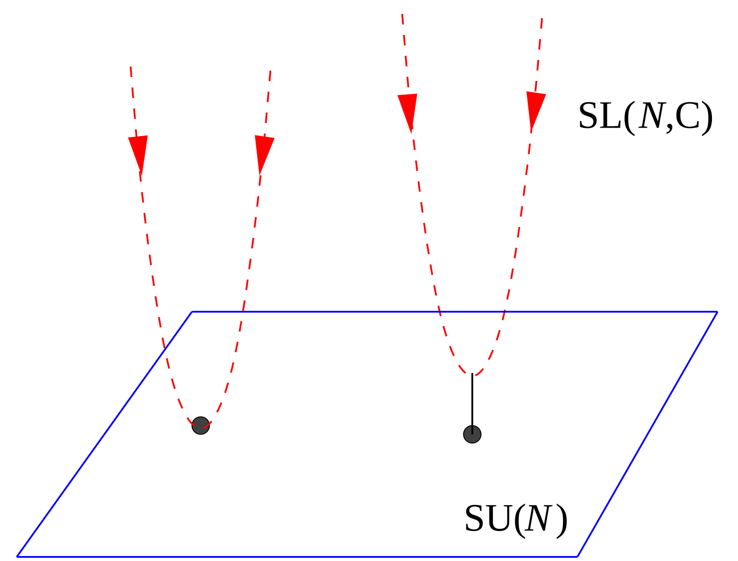
what is f_a^k? $\qquad \Omega_k = e^{-\alpha f_a^k \lambda_a} \qquad \mathrm{d}' - \mathrm{d} = -\alpha/N(f_a^k)^2 + \ldots$

- choose f_a^k as the gradient of the unitarity norm

$$f_a^k = 2\mathrm{Tr}\,\lambda_a \left(U_k U_k^\dagger - U_{k-1}^\dagger U_{k-1} \right)$$

- if $U \in$ SU(N): $f_a^k = 0$, $\mathrm{d} = 0$, no effect

cooling brings the links as close as possible to SU(N)



Gauge cooling

- simple example: one-link model 1303.6425

$$S = \frac{1}{N}\mathrm{Tr}\, U \qquad\qquad U \to \Omega U \Omega^{-1}$$

$$\mathrm{d} = \frac{1}{N}\mathrm{Tr}\,\left(UU^\dagger - 1\!\!1\right) \qquad\qquad f_a = 2\mathrm{Tr}\,\lambda_a\left(UU^\dagger - U^\dagger U\right)$$

- note: $c = \mathrm{Tr}\, U/N, \;\; c^* = \mathrm{Tr}\, U^\dagger/N$ invariant under cooling
- cooling dynamics:

$$\mathrm{d}' - \mathrm{d} \equiv \dot{\mathrm{d}} = -\frac{\alpha}{N} f_a^2 = -\frac{16\alpha}{N}\mathrm{Tr}\, UU^\dagger[U, U^\dagger]$$

- in SU(2)/SL(2,$\mathbb{C}$):

$$\dot{\mathrm{d}} = -8\alpha\left(\mathrm{d}^2 + 2\left(1 - |c|^2\right)\mathrm{d} + c^2 + c^{*2} - 2|c|^2\right)$$

Gauge cooling

SU(2)/SL(2,$\mathbb{C}$) one-link model

$$\dot{\text{d}} = -8\alpha\left(\text{d}^2 + 2\left(1-|c|^2\right)\text{d} + c^2 + c^{*2} - 2|c|^2\right)$$

- $c = \frac{1}{2}\mathrm{Tr}\,U, \quad c^* = \frac{1}{2}\mathrm{Tr}\,U^\dagger$ invariant under cooling
- if $c = c^*$: U gauge equivalent to SU(2) matrix

$$\dot{\text{d}} = 8\alpha(\text{d} + 2 - 2c^2)\text{d} \qquad\qquad \text{d}(t) \sim e^{-16\alpha(1-c^2)t} \to 0$$

- if $c \neq c^*$: U not gauge equivalent to SU(2) matrix

$$\text{d}(t) \to \text{d}_0 = |c|^2 - 1 + \sqrt{1 - c^2 - c^{*2} + |c|^4} > 0$$

minimal distance from SU(2)
reached exponentially fast
power law in case of many links

Langevin with gauge cooling

complex Langevin dynamics with gauge cooling:

- alternate CL updates with gauge cooling updates
- monitor unitarity norm
- stay fairly close to SU(N)

models

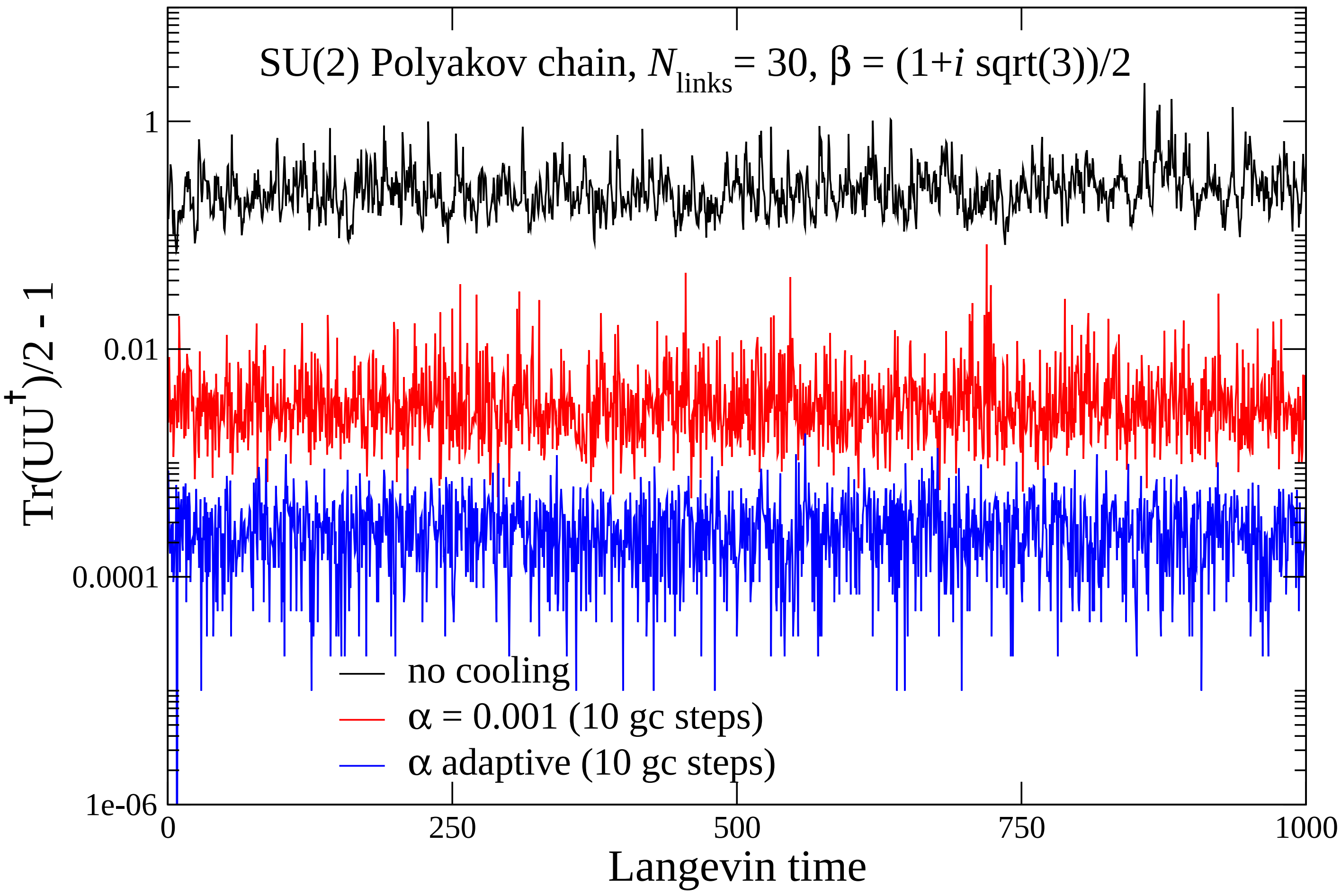
- Polyakov chain (exactly solvable)

$$S = \beta_1 \mathrm{Tr}\, U_1 \dots U_{N_\ell} + \beta_2 \mathrm{Tr}\, U_{N_\ell}^{-1} \dots U_1^{-1} \qquad\qquad \beta_{1,2} \in \mathbb{C}$$

- heavy dense QCD `ES, DS & IOS 12, GA, Attanasio, Jäger, Sexty 16`
- full QCD `Dénes Sexty 13`

Langevin with gauge cooling

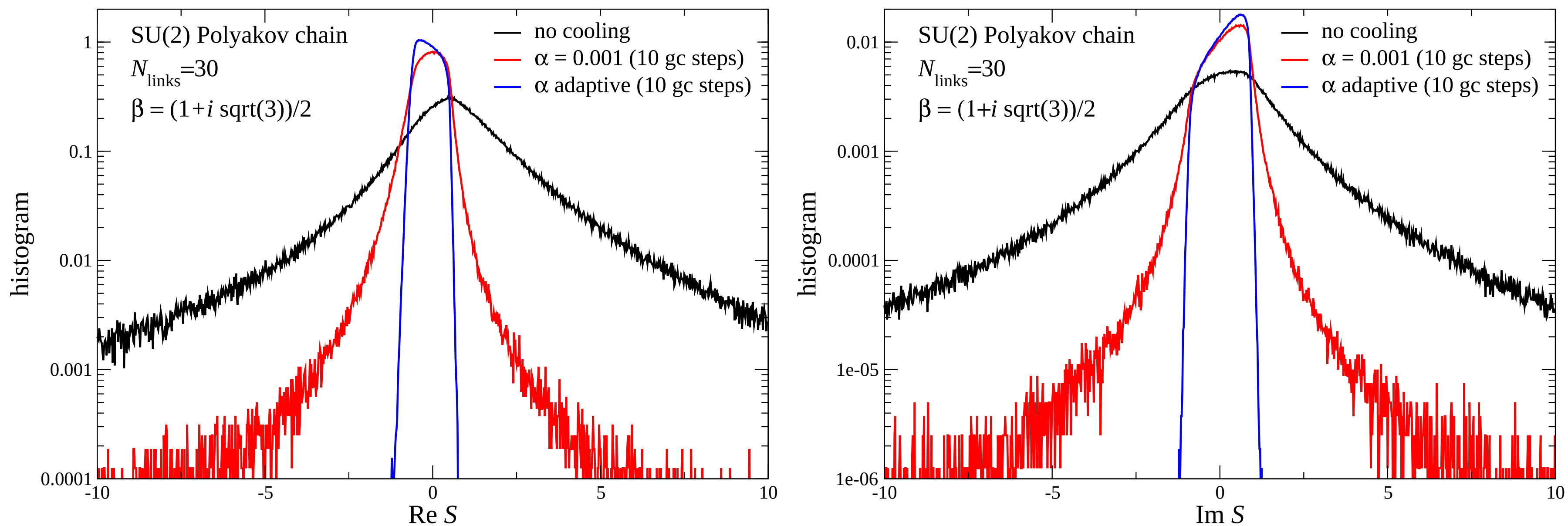
SU(2) Polyakov loop model 1303.6425



evolution of unitarity norm

Langevin with gauge cooling

SU(2) Polyakov loop model



histograms of observables

- without cooling: broad distributions, no rapid decay
- with some cooling: reduced
- with sufficient adaptive cooling: narrow distributions

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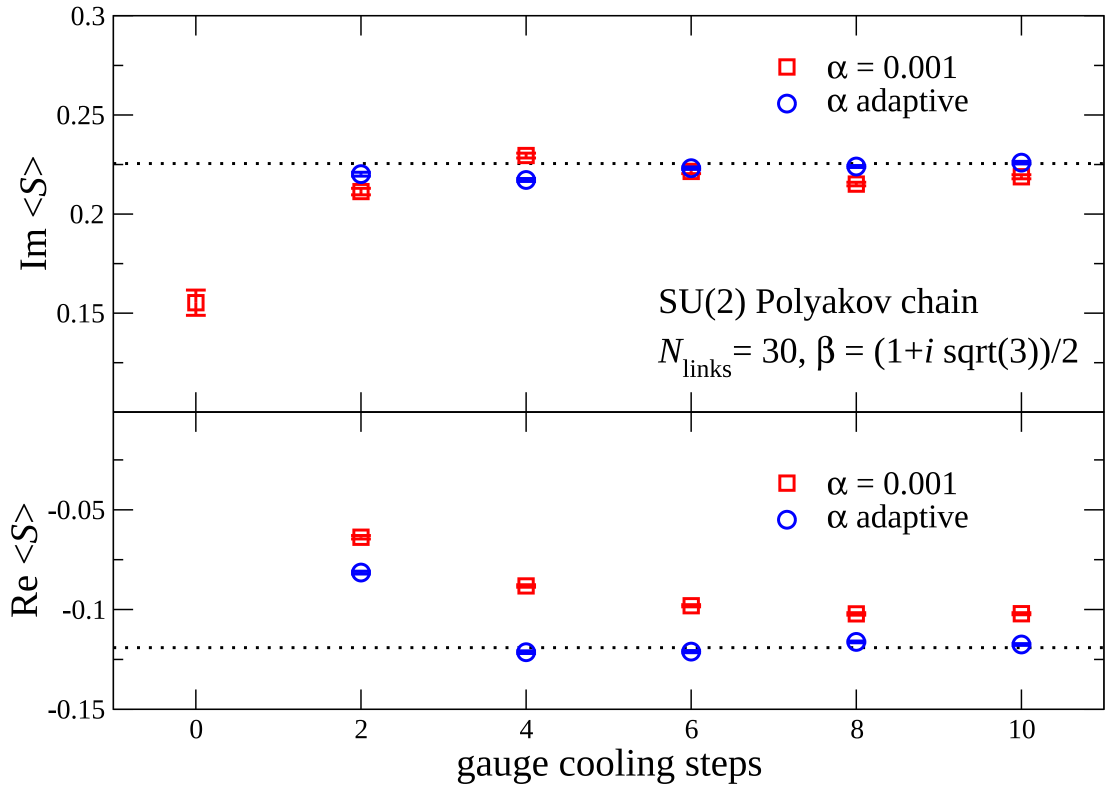

- observables depend on gauge cooling
- exact results are reproduced when distributions are narrow and unitarity norm close to 0

Langevin with gauge cooling

in QCD:

- unitary submanifold very unstable
- gauge cooling essential

many things to sort out

- combine with dynamical stabilisation Attanasio & Jäger
- non-holomorphicity due to $\log \det \Rightarrow$ poles in Langevin drift 1701.02322
- boundary terms at infinity and around poles
- heavy dense QCD under control
- full QCD not yet

Outlook

towards the phase diagram of QCD from the lattice

- various ideas under investigation
- new algorithms: implementation in simpler models
- complexified manifolds
- interplay with thimbles and variations thereof

- applications to other systems, e.g. non-relativistic models, very promising
- perhaps some technical complications less relevant