Complex Langevin dynamics: distributions and gauge theories

Gert Aarts

Swansea University
Prifysgol Abertawe

QCD phase diagram

QCD partition function

$$Z = \int DU\, D\bar{\psi} D\psi\, e^{-S_{\mathrm{YM}} - S_{\mathrm{F}}} = \int DU\ \det D\, e^{-S_{\mathrm{YM}}}$$

at nonzero quark chemical potential

$$[\det D(\mu)]^* = \det D(-\mu^*)$$

- fermion determinant is complex
- straightforward importance sampling not possible
- sign problem

$\Rightarrow$ phase diagram has not yet been determined non-perturbatively

Outline

- complex Langevin dynamics: exploring a complexified field space
- distributions in simple models
- connection with Lefschetz thimbles
- gauge theories: from SU(N) to SL($N, \mathbb{C}$)
- summary and outlook

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

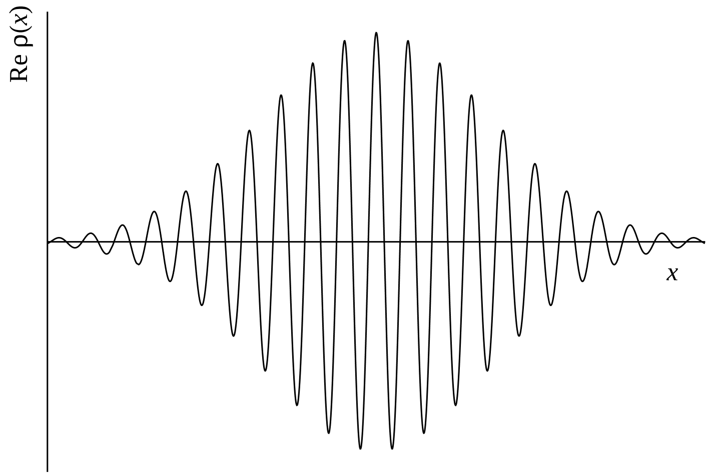
radically different approach:

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

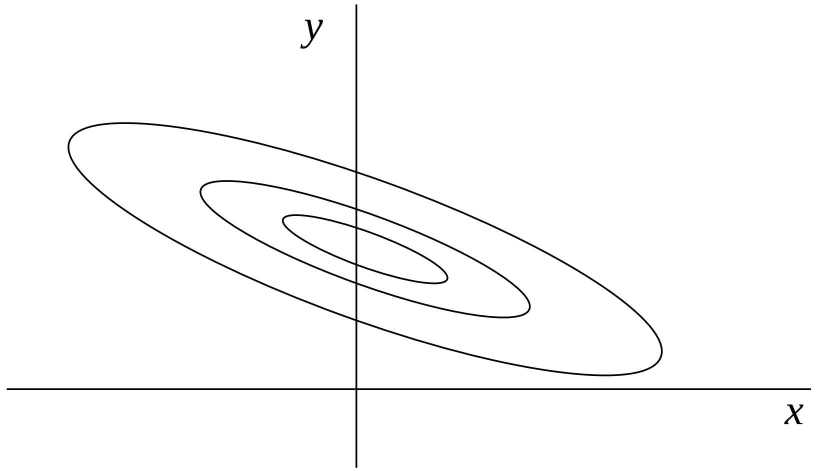
Complexified field space

complex weight $\rho(x)$

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

Complex Langevin dynamics

does it work?

- for real actions: stochastic quantization Parisi & Wu 81
- equivalent to path integral quantization

Damgaard & Hüffel, Phys Rep 87

- for complex actions: no formal proof
- troubled past: “disasters of various degrees”

Ambjørn et al 86

nevertheless, recent examples in which CL

- can handle severe sign and Silver Blaze problems
- gives the correct result
- analytical understanding under control
- first results for gauge theories and QCD

Complex Langevin dynamics

various scattered results since mid 1980s

here:

finite density results obtained with Nucu Stamatescu, Erhard Seiler, Frank James, Denes Sexty, Lorenzo Bongiovanni, Jan Pawlowski, Pietro Giudice, Kim Splittorff

0807.1597 [GA, IOS]

0810.2089, 0902.4686 [GA]

0912.3360 [GA, ES, IOS]

0912.0617, 1101.3270 [GA, FJ, ES, IOS]

1005.3468, 1112.4655 [GA, FJ]

1006.0332 [GA, KS]

1211.3709 [ES, DS, IOS]

1212.5231 [GA, FJ, JP, ES, DS, IOS]

1306.3075 [GA, PG, ES]

1307.7748 [DS] 1308.4811 [GA]

1311.1056 [GA, LB, IOS, ES, DS]

reviews: 1302.3028 [GA], 1303.6425 [GA, LB, IOS, ES, DS]

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

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

- Fokker-Planck hamiltonian:

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

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

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

Complex Langevin dynamics

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

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

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

- 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?

Field theory

scalar field:

- (discretized) Langevin dynamics in “fifth” time direction

$$\phi_x(n+1) = \phi_x(n) + \epsilon K_x(n) + \sqrt{\epsilon}\eta_x(n)$$

- drift: $K_x = -\delta S[\phi]/\delta\phi_x$
- Gaussian noise: $\langle\eta_x(n)\rangle = 0 \quad \langle\eta_x(n)\eta_{x'}(n')\rangle = 2\delta_{xx'}\delta_{nn'}$

Field theory

scalar field:

- (discretized) Langevin dynamics in "fifth" time direction

$$\phi_x(n+1) = \phi_x(n) + \epsilon K_x(n) + \sqrt{\epsilon}\eta_x(n)$$

- drift: $K_x = -\delta S[\phi]/\delta\phi_x$
- Gaussian noise: $\langle \eta_x(n) \rangle = 0 \quad \langle \eta_x(n)\eta_{x'}(n') \rangle = 2\delta_{xx'}\delta_{nn'}$

gauge/matrix theories:

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

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

- drift: $K_a = -D_a(S_B + S_F) \qquad S_F = -\ln\det M$
- complex action: $K^\dagger \neq K \Leftrightarrow U \in$ SL($N, \mathbb{C}$)

Results

even without rigorous mathematical proof
many promising results at nonzero μ:

- 1d QCD
- 3d SU(3) spin models
- 4d Bose gas (severe sign and Silver Blaze problem)
- heavy dense QCD

however, also notable failures

- 3d XY model at nonzero μ

also problems for

- Minkowski integrals, e^{iS}

Berges, Borsanyi, Stamatescu, Sexty 05 - 08

Distributions

emerging insight: 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 $\mu \sim 0$?

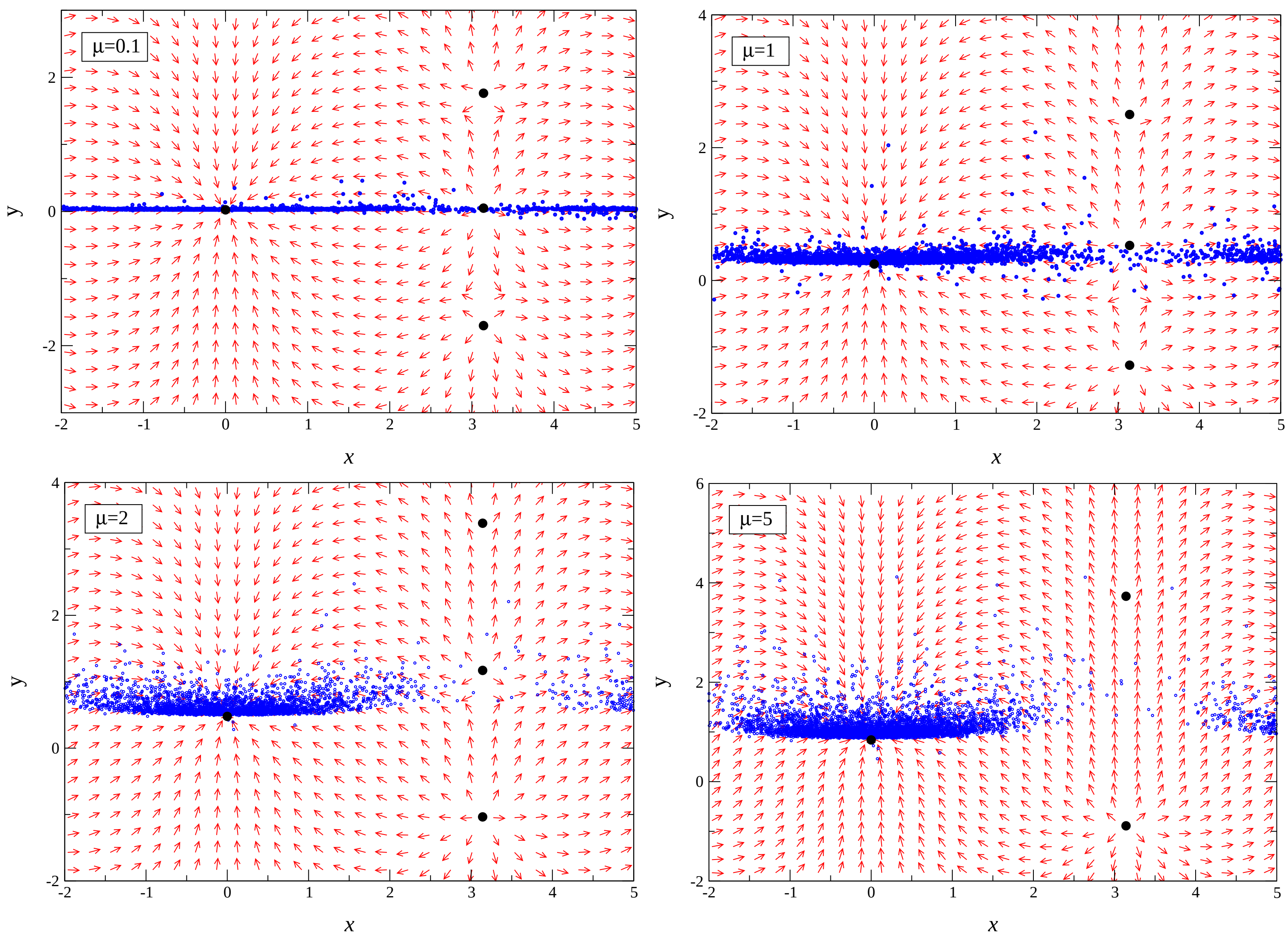
  `GA, FJ, JP, ES, DS & IOS 12`

study with histograms, scatter plots, flow

Distributions

distribution in well-behaved example

GA & IOS 08



One-dimensional QCD

- exactly solvable   Gibbs 86, Bilic & Demeterfi 88
- phase quenched: transition at $\mu = \mu_c$, full: no transition

$$\boxed{\text{severe sign problem when } |\mu| > |\mu_c|}$$

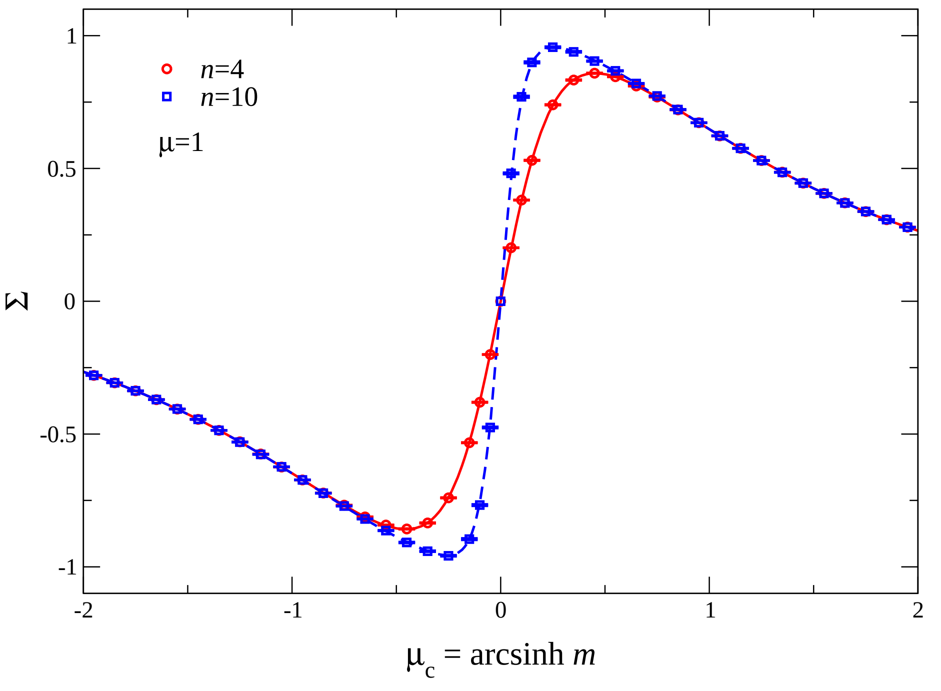
- chiral condensate:
  write as integral over spectral density

$$\Sigma = \int d^2 z \, \frac{\rho(z;\mu)}{z+m} \qquad \mu_c = \text{arcsinh}\, m$$

- $\rho(z;\mu)$ complex and oscillatory   Ravagli & Verbaarschot 07
- condensate independent of μ: Silver Blaze
- solve with complex Langevin   GA & Splittorff 10

One-dimensional QCD

- exact results reproduced
- discontinuity at $\mu_c = 0$ in thermodynamic limit $n \to \infty$



- sign problem severe when $|\mu_c| < |\mu|$
- condensate independent of μ: Silver Blaze

One-dimensional QCD

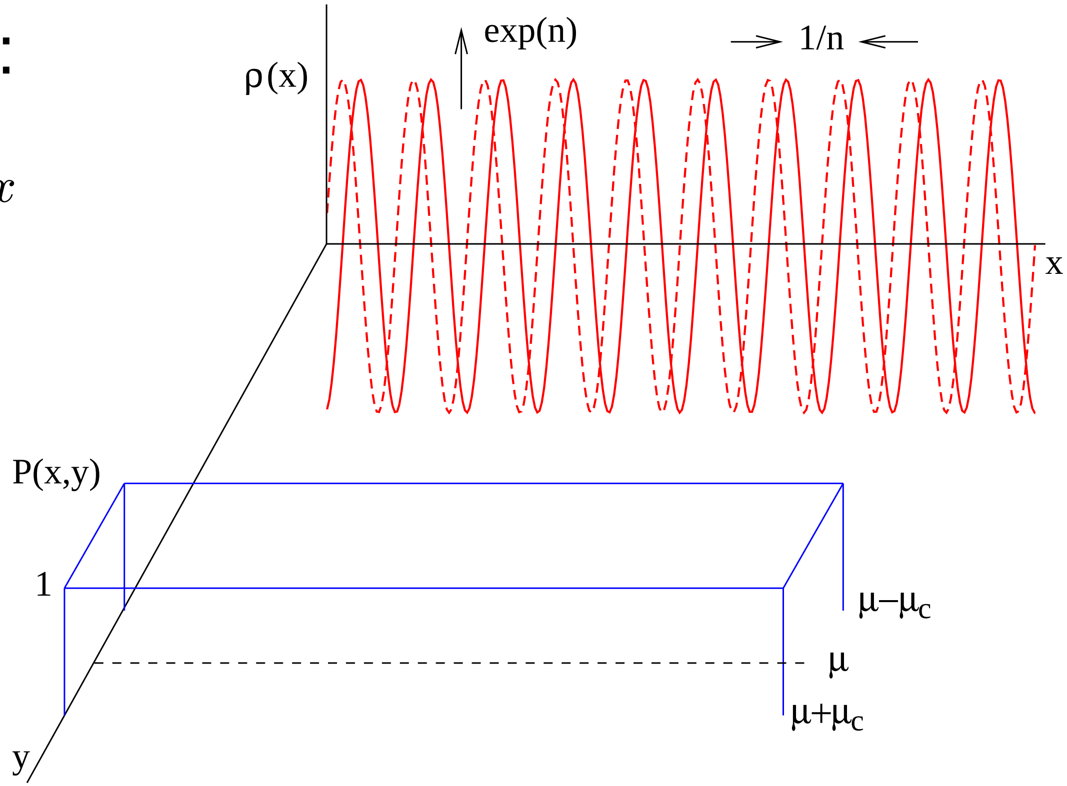
elegant analytical solution:

- original distribution:

  $$\rho(x) \sim e^{n(\mu-\mu_c)} e^{inx}$$

  when $n \to \infty$

- real distribution sampled by complex Langevin:



$$P(x,y) = \begin{cases} 1 & \mu - \mu_c < y < \mu + \mu_c \\ 0 & \text{elsewhere} \end{cases}$$

Quartic model

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

often used toy model: complex mass parameter $\sigma = A + iB$

GA, PG & ES 13

essentially analytical proof:

- CL gives correct result for all observables $\langle x^n \rangle$ when $A > 0$ and $A^2 > B^2/3$
- based on properties of the distribution $P(x,y)$
- $P(x,y) = 0$ outside strip: $|y| > y_-$

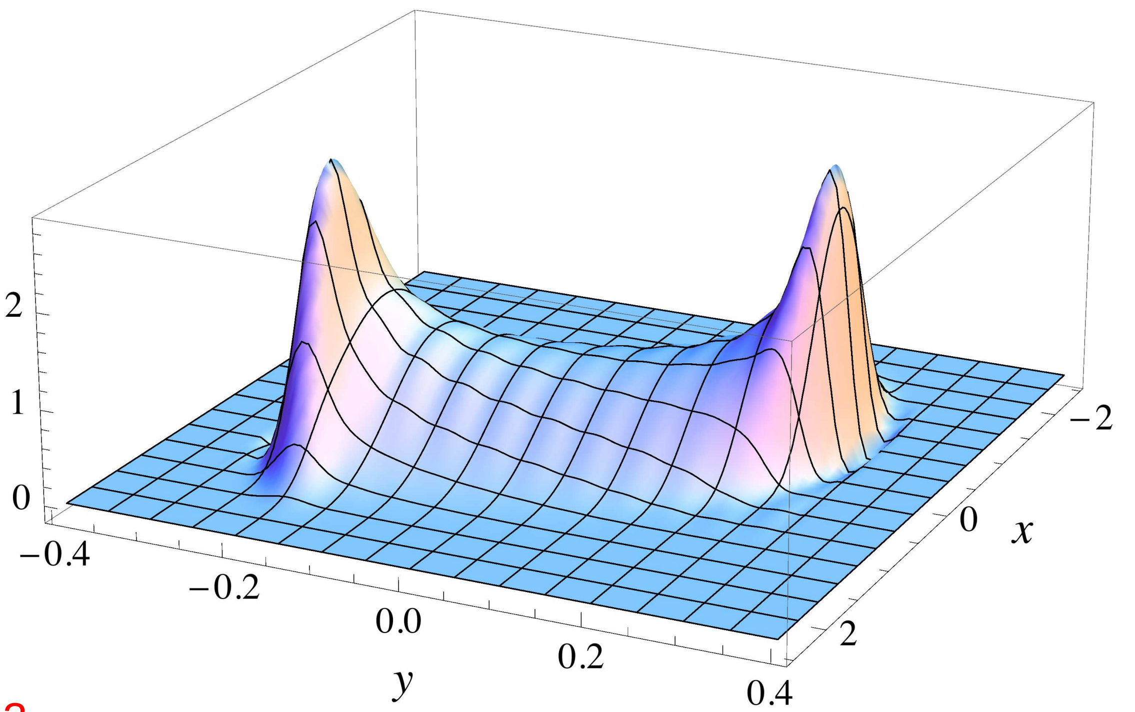
$$y_- = \frac{1}{2\lambda}\left(A - \sqrt{A^2 - B^2/3}\right)$$

- follows from FPE

Quartic model

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

- numerical solution of FPE for $P(x,y)$
  $\sim 150^2 \times 150^2$ matrix problem
- distribution is localised in a strip around real axis



GA, PG & ES 13

Quartic model

interesting connection to Lefschetz thimbles Witten 10

Cristoforetti, Di Renzo, Mukherjee & Scorzato 12, 13

Fujii, Honda, Kato, Kikukawa, Komatsu & Sano 13

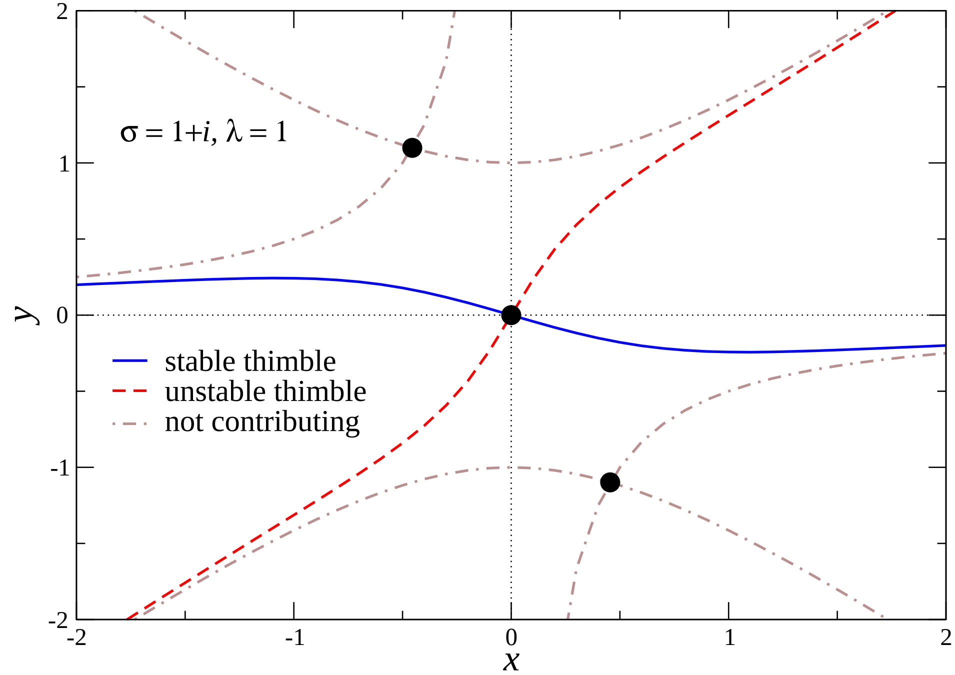
- generalisation of steepest descent
- integrate along path in complex plane where $\mathrm{Im}\, S(z) =$ cst, the thimble $\mathcal{J}$
- residual sign problem due to curvature of thimble

$$Z = e^{-i\mathrm{Im}\, S_{\mathcal{J}}} \int_{\mathcal{J}} dz\, e^{-\mathrm{Re}\, S(z)}$$
$$= e^{-i\mathrm{Im}\, S_{\mathcal{J}}} \int ds\, J(s) e^{-\mathrm{Re}\, S(z(s))}$$

with complex Jacobian $J(s) = z'(s) = x'(s) + iy'(s)$

Quartic model

- thimbles can be computed analytically
- pass through stationary points $\partial_z S = 0$ & $\mathrm{Im}\, S(z) = $ cst

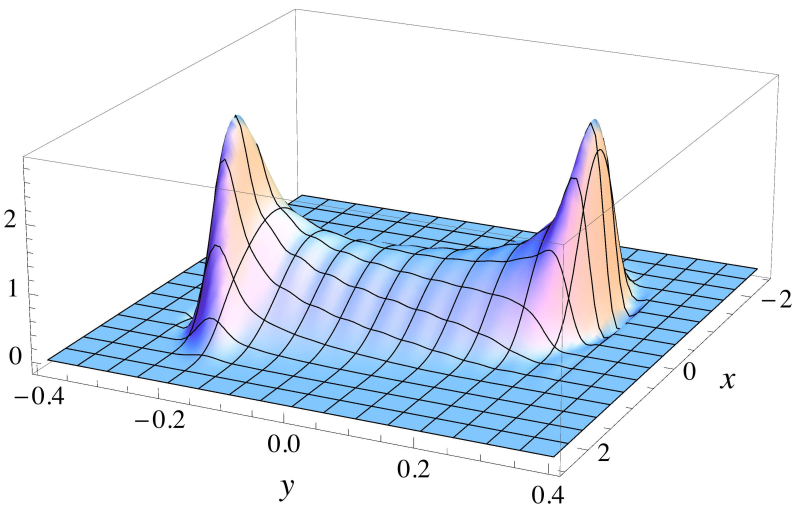


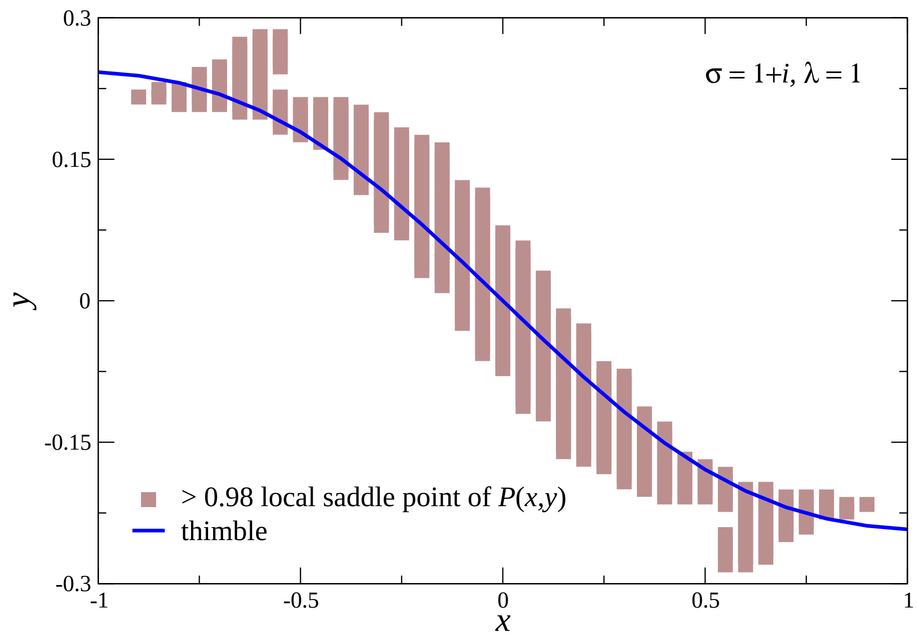
- 3 stationary points: only 1 thimble (for $A > 0$)
- integrating along thimble gives correct result, with inclusion of complex Jacobian

Quartic model

compare thimble and FP distribution $P(x, y)$

GA 13





- thimble and $P(x, y)$ follow each other
- however, weight distribution quite different

intriguing result: CLE finds the thimble – is this generic?

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 ($a = 1, \dots N^2 - 1$)

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

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 ($a = 1, \ldots N^2 - 1$)

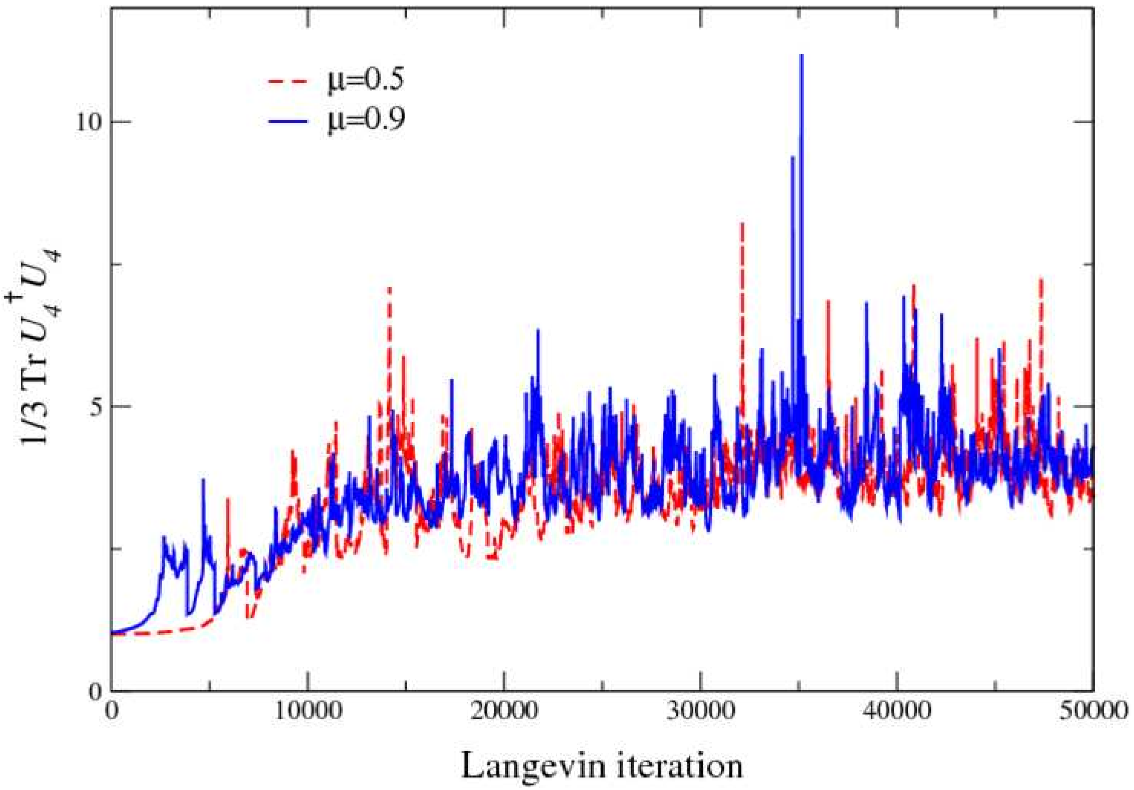
- drift: $K_a = -D_a(S_B + S_F) \qquad S_F = -\ln\det M$
- complex action: $K^\dagger \neq K \Leftrightarrow U \in$ SL($N, \mathbb{C}$)
- deviation from SU(N): unitarity norms

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

Gauge theories

deviation from SU(3): unitarity norm GA & IOS 08

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



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 12

GA, LB, ES, DS & IOS 13

Gauge cooling

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

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

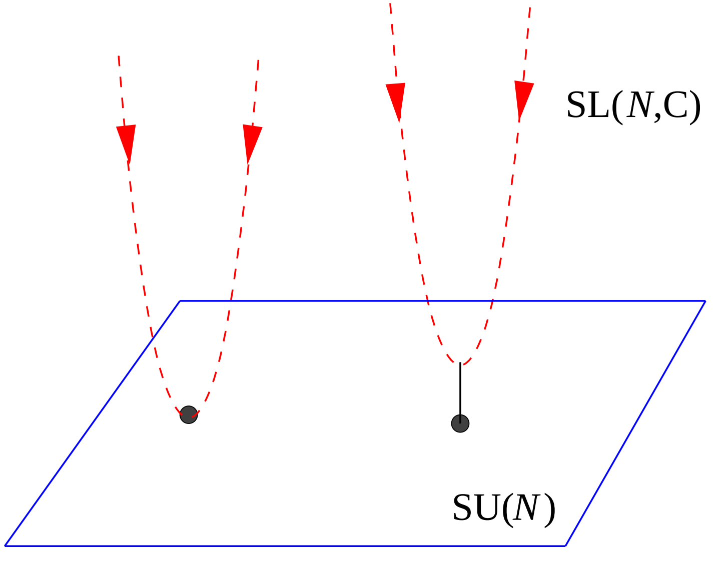
unitarity norm: distance $\qquad \mathrm{d} = \sum_k \frac{1}{N} \mathrm{Tr}\left(U_k U_k^\dagger - \mathbb{1}\right)$

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

linearise

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

reduce distance from SU(N)



Gauge cooling

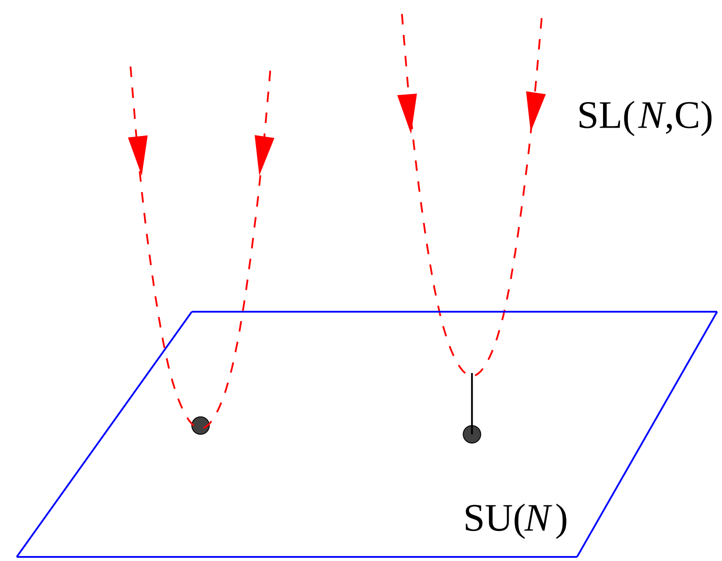
what is f_a^k? $\qquad \Omega_k = e^{-\alpha f_a^k \lambda_a} \qquad d' - d = -\alpha/N(f_a^k)^2 + \ldots$

- 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): $f_a^k = 0$, $d = 0$, no effect

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



Gauge cooling

- simple example: one-link model

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

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

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

- cooling dynamics:

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

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

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

Gauge cooling

SU(2)/SL(2,ℂ) one-link model

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

- $c = \frac{1}{2}\text{Tr}\, U, \quad c^* = \frac{1}{2}\text{Tr}\, U^\dagger$ 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

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

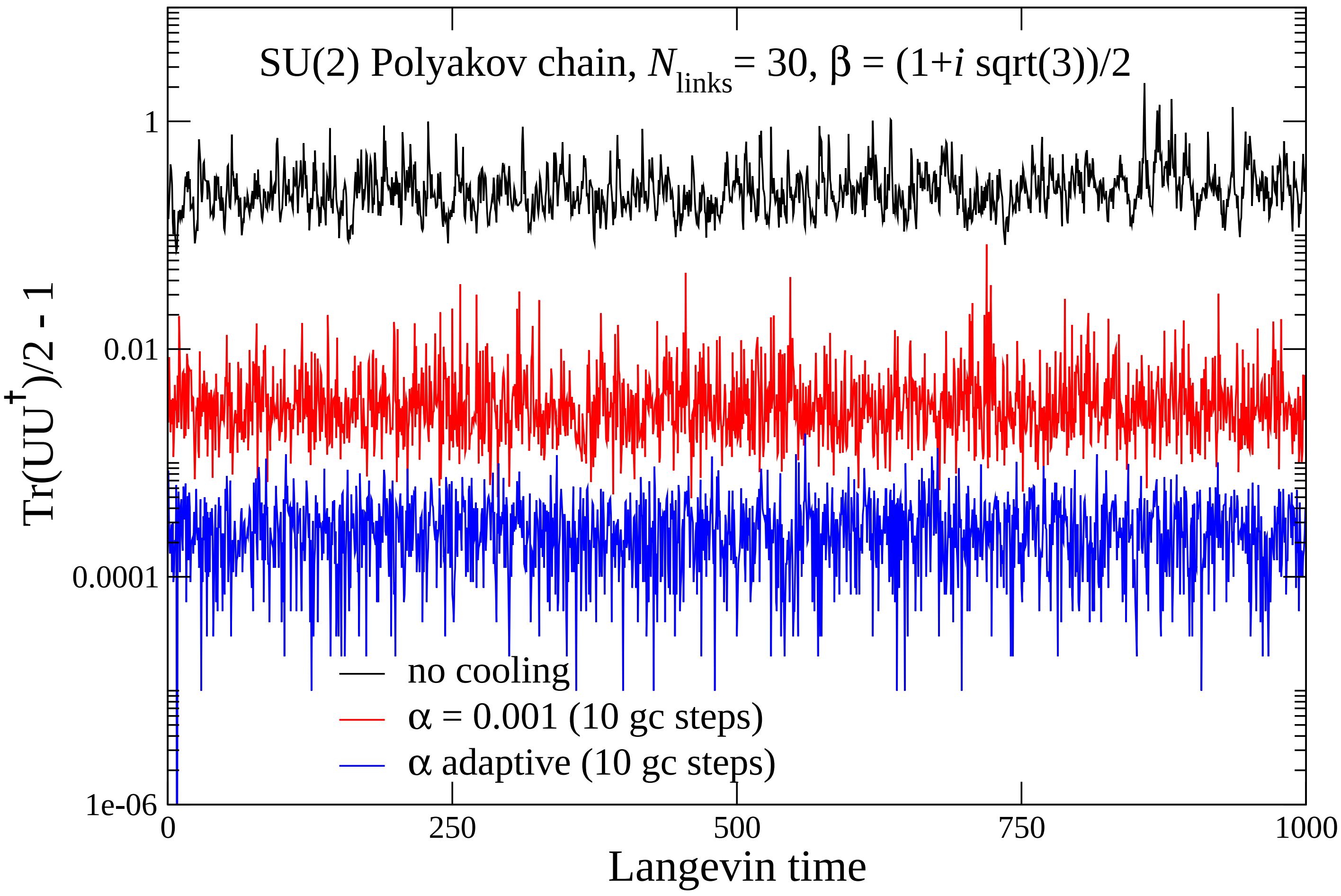
- Polyakov chain (exactly solvable)

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

- heavy dense QCD ES, DS & IOS 12
- full QCD Denes Sexty 1307.7748
- SU(3) with a θ-term GA, LB, ES, DS, IOS 1311.1056

Langevin with gauge cooling

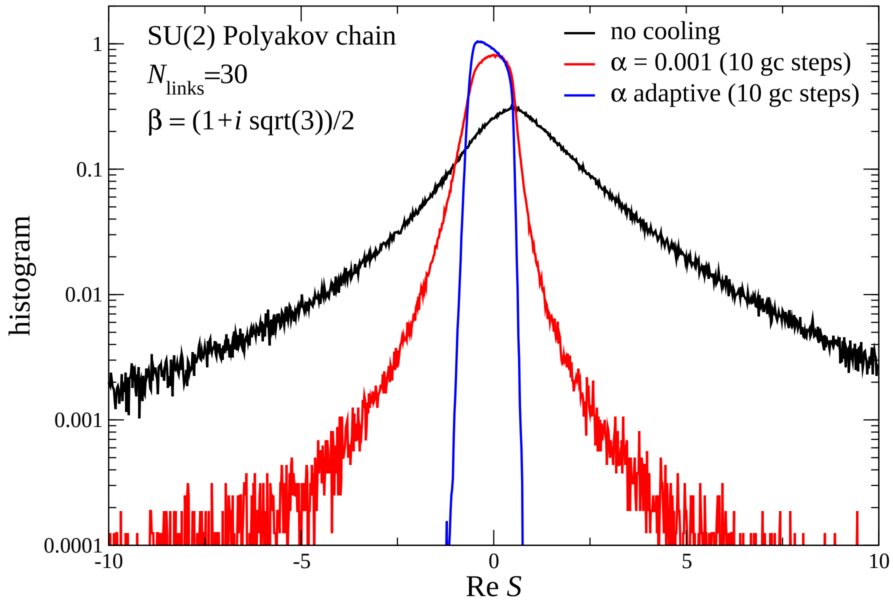
SU(2) Polyakov loop model GA, LB, ES, DS & IOS 13

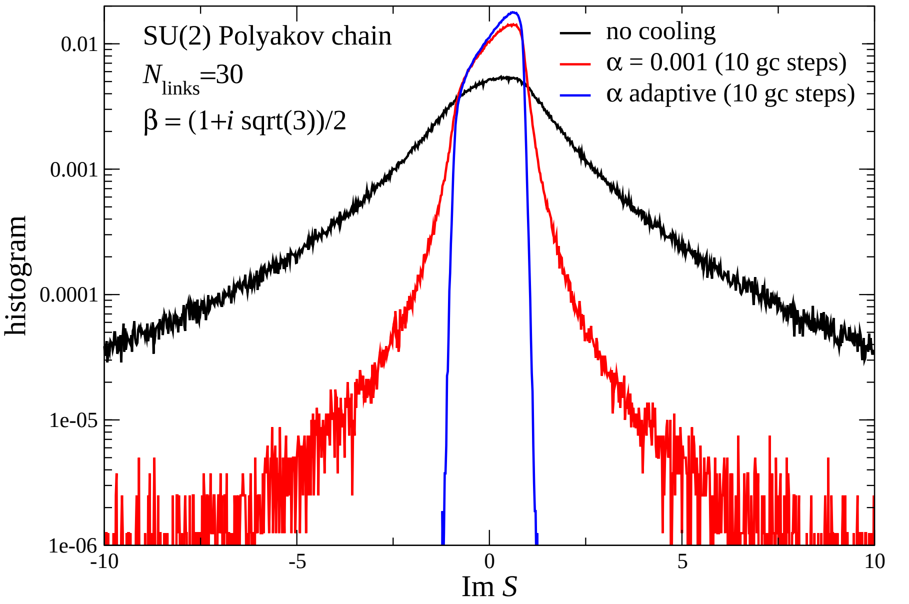


evolution of unitarity norm

Langevin with gauge cooling

SU(2) Polyakov loop model



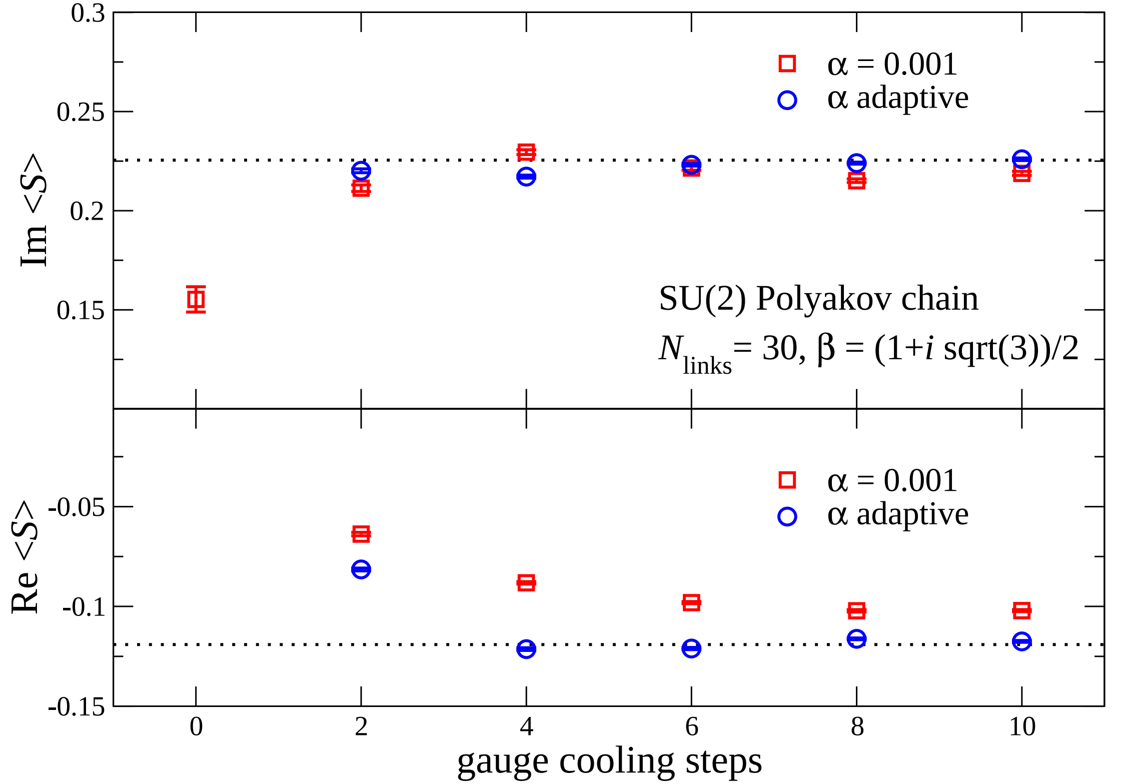


histograms of observables

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

Langevin with gauge cooling

SU(2) Polyakov loop model



- 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
- first results promising `Denes Sexty 1307.7748`

many things to sort out

- cooling not effective at small $\beta \lesssim 5.7$
- larger lattices required
- fermion matrix inversion
- stepsize dependence
- $\dots$

here: SU(3) with a θ term `GA, LB, ES, DS, IOS 1311.1056`

SU(3) with a θ term

pure SU(3) Yang-Mills theory (no fermions)

$$S = S_{\mathrm{YM}} - i\theta Q \qquad\qquad Q = \frac{g^2}{64\pi^2}\int d^4x\, F^a_{\mu\nu}\tilde{F}^a_{\mu\nu}$$

on the lattice:

$$S = S_W - i\theta_L \sum_x q_L(x) \qquad\qquad q_L(x) = \text{discretised lattice version}$$

- θ_L bare parameter, requires renormalisation
- lattice $Q_L = \sum_x q_L$ is not topological (top. cooling)
- complex action for real θ_L, real action for imaginary θ_L

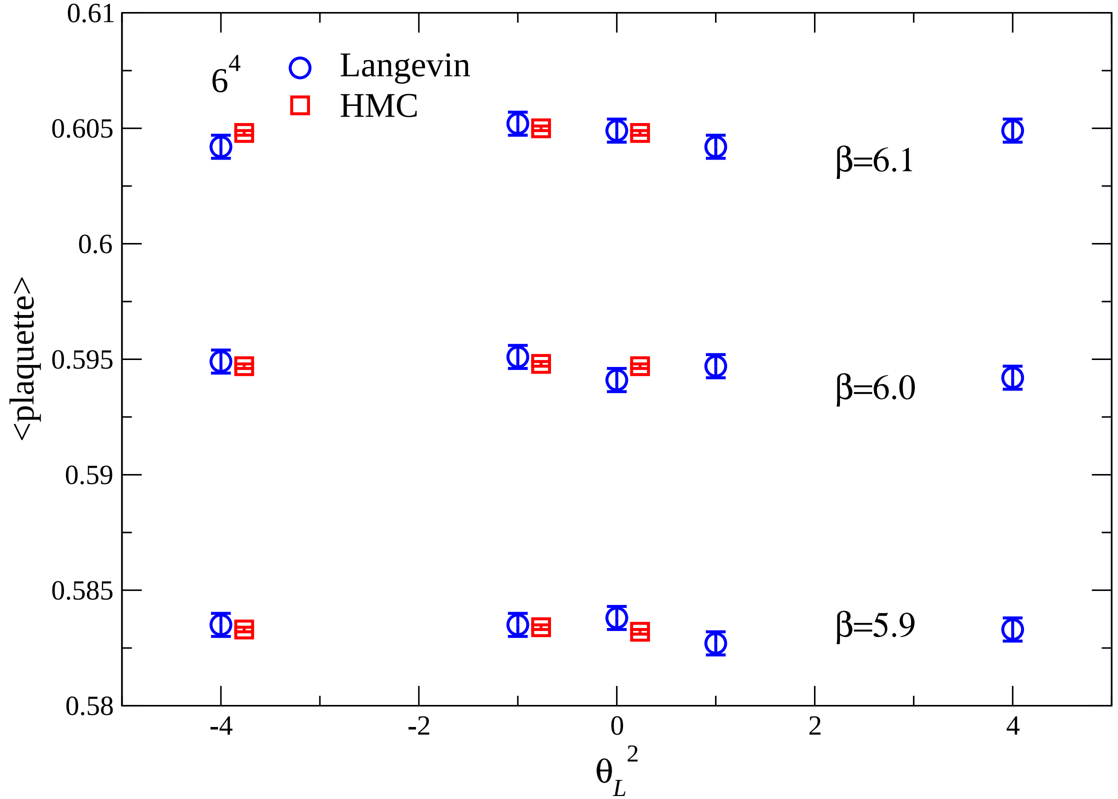
imaginary θ_L: real Langevin and hybrid Monte Carlo (HMC)

real θ_L: use complex Langevin

SU(3) with a θ term

very preliminary results: 6^4 lattice, $\theta_L^2 = 0, \pm 1, \pm 4$

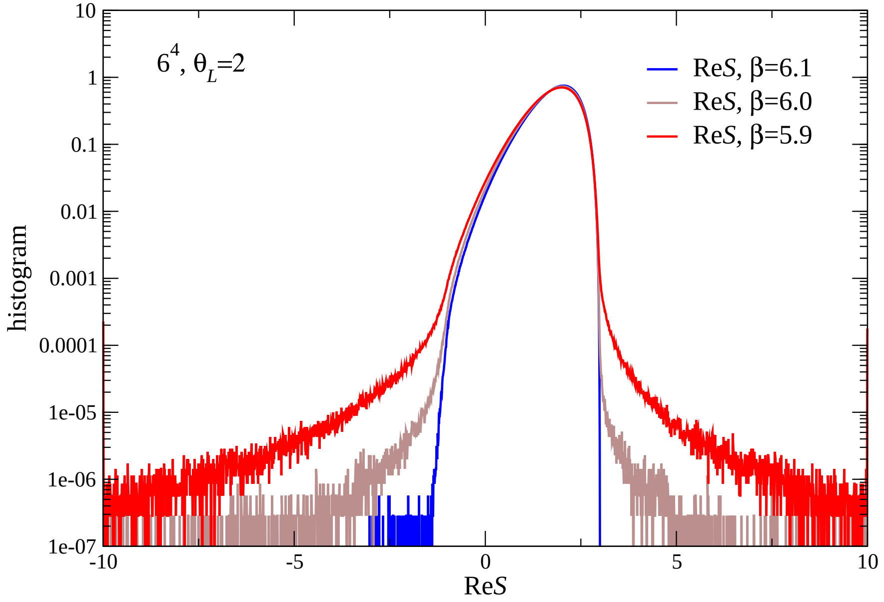
test of analyticity in θ_L^2: $\langle$plaquette$\rangle$

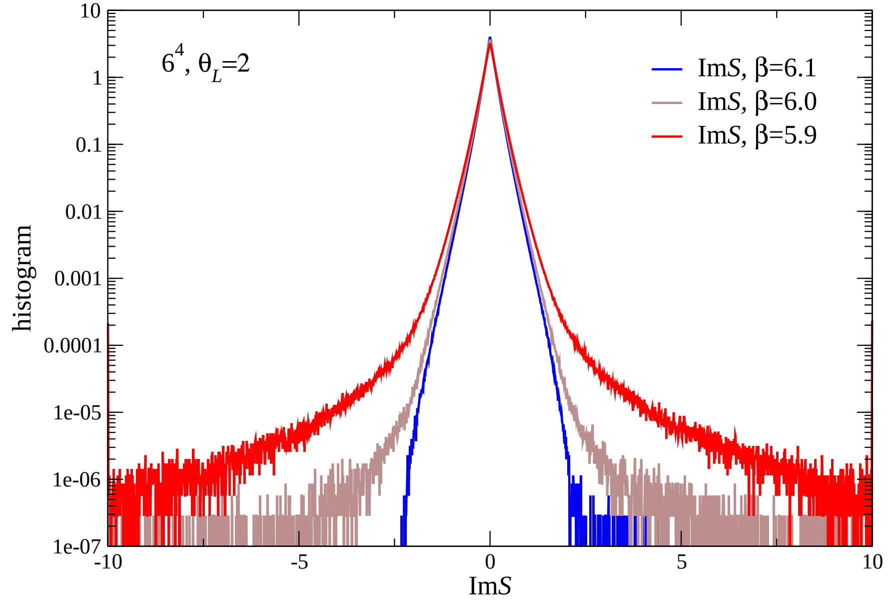


no θ_L dependence: smooth analytic behaviour
(as expected)

SU(3) with a θ term

very preliminary results: 6^4 lattice, $\theta_L^2 = 0, \pm 1, \pm 4$





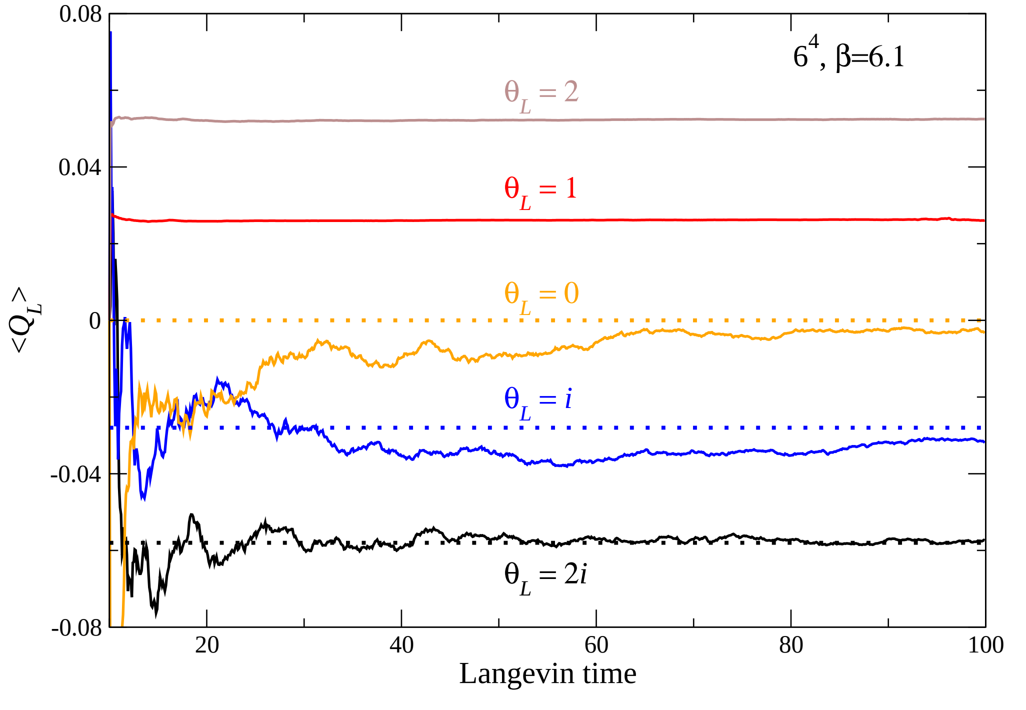
Re S Im S

histograms: better localisation at larger β values

SU(3) with a θ term

topological charge:

- θ_L real/imaginary: $\langle Q_L \rangle$ imaginary/real
- small θ_L: linear dependence $\langle q_L \rangle = i\theta_L \chi_L + \mathcal{O}(\theta_L^3)$
  χ_L lattice topological susceptibility



running average: preliminary result agrees with expectation

Summary and outlook

complex Langevin dynamics can handle

- sign problem
- Silver Blaze problem
- phase transition
- thermodynamic limit

in a variety of theories, but correct result not guaranteed

so far

- better mathematical and practical understanding
- connection with Lefschetz thimbles
- gauge cooling for SU(N) gauge theories
- first application to QCD and θ term

lots of work to do!

Helmholtz Alliance

Extremes of Density and Temperature: Cosmic Matter in the Laboratory

ExtreMe Matter Institute EMMI

EMMI Workshop

SIGN 2014

International Workshop on the Sign Problem in QCD and beyond

February 18 - 21, 2014, GSI Darmstadt, Germany

Topics

- QCD at nonzero density
- strongly correlated fermions
- dual formulations
- quantum simulators
- new algorithms

Organizers

Gert Aarts, Swansea University

Owe Philipsen, Frankfurt University

Information

http://www.gsi.de/emmi/workshops

More about EMMI

www.gsi.de/emmi

GSI

HELMHOLTZ ASSOCIATION

EMMI