Complex Langevin dynamics and the sign problem

GGI 2012

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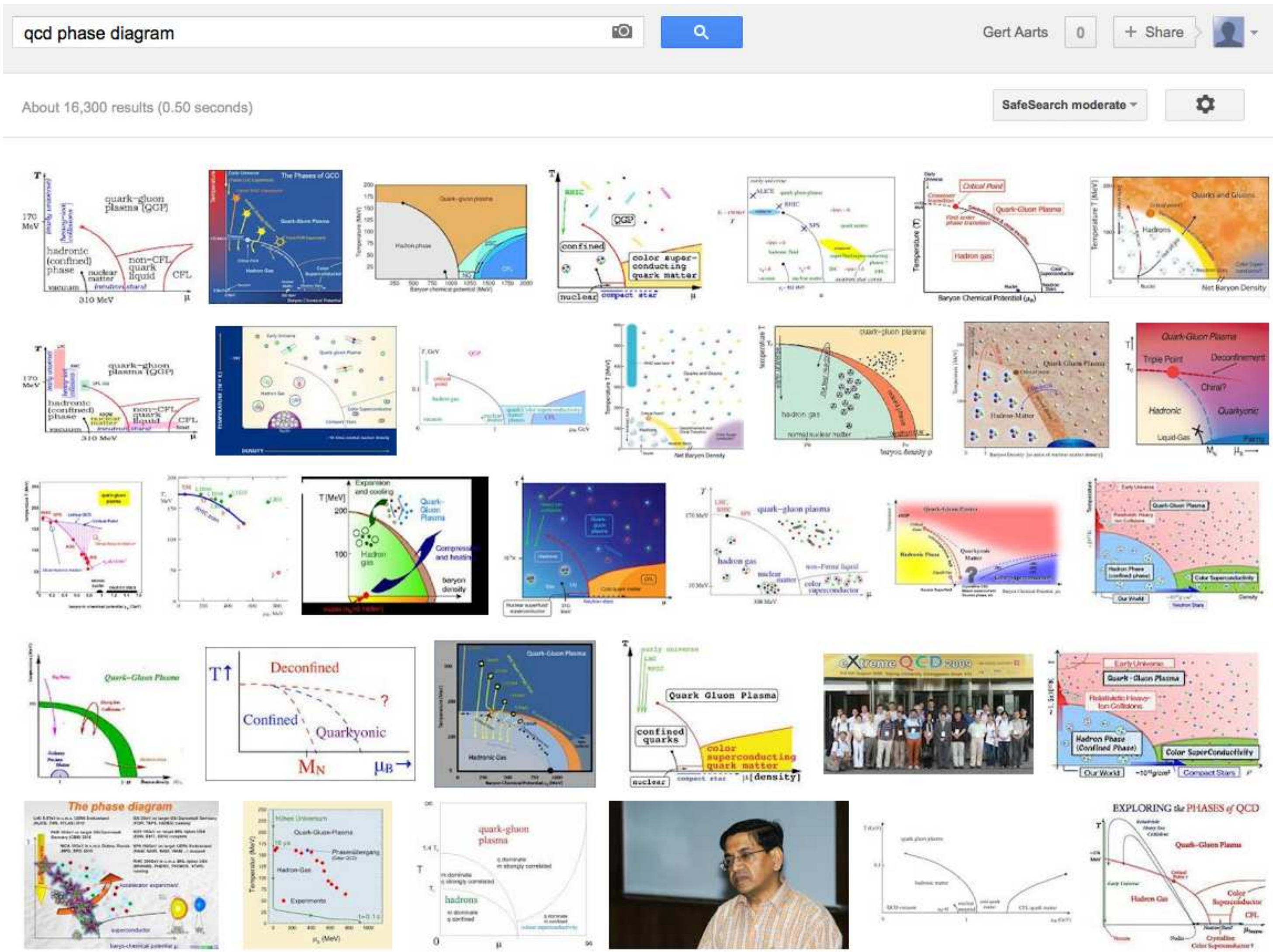
QCD phase diagram



QCD phase diagram?

at finite baryon chemical potential: complex weight

- straightforward importance sampling not possible
- overlap problem

various possibilities:

- preserve overlap as best as possible
- use approximate methods at small μ
- do something radical:
  - rewrite partition function in other dof
  - explore field space in a different way
  - . . .

Outline

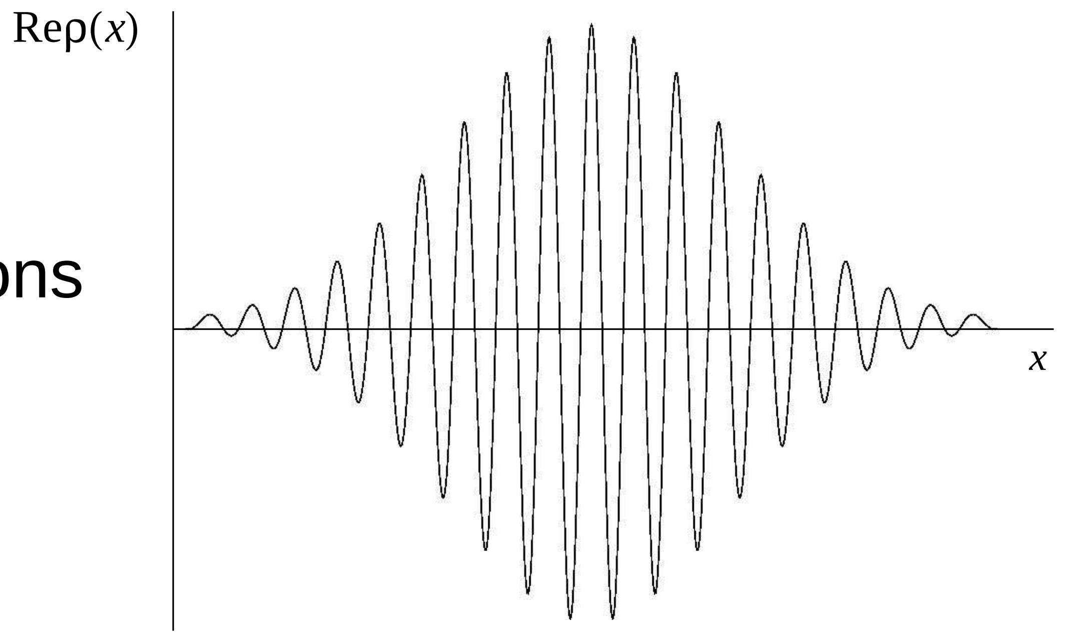
- into complex plane
- reminder: real vs. complex Langevin dynamics
- troubled past: stability and convergence

- SU(3) spin model . . .
- . . . versus XY model
- Haar measure
- lessons? exploit freedom?

Overlap problem

- configurations differ in an essential way from those obtained at $\mu = 0$ or with $|\det M|$
- 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

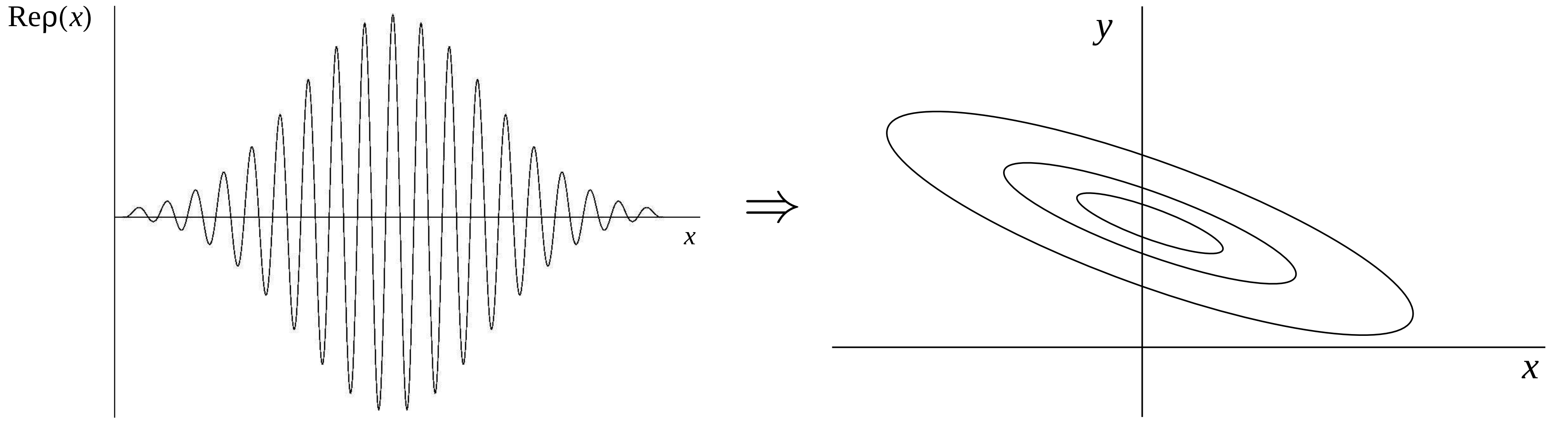
- lesson: don't be real(istic), be more imaginative

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?



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

$\Rightarrow$ solution of stochastic process

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

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

- 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?

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

GA, Frank James, Erhard Seiler,
Nucu Stamatescu (& Denes Sexty) 08-now
GA & Kim Splittorff 10

Troubled past

1. numerical problems: runaways, instabilities

   $\Rightarrow$ adaptive stepsize

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

   `GA, James, Seiler & Stamatescu 09`

   `a la Ambjorn et al 86`

2. theoretical status unclear

   $\Rightarrow$ detailed analyis, identified necessary conditions

   `GA, FJ, ES & IOS 09-12`

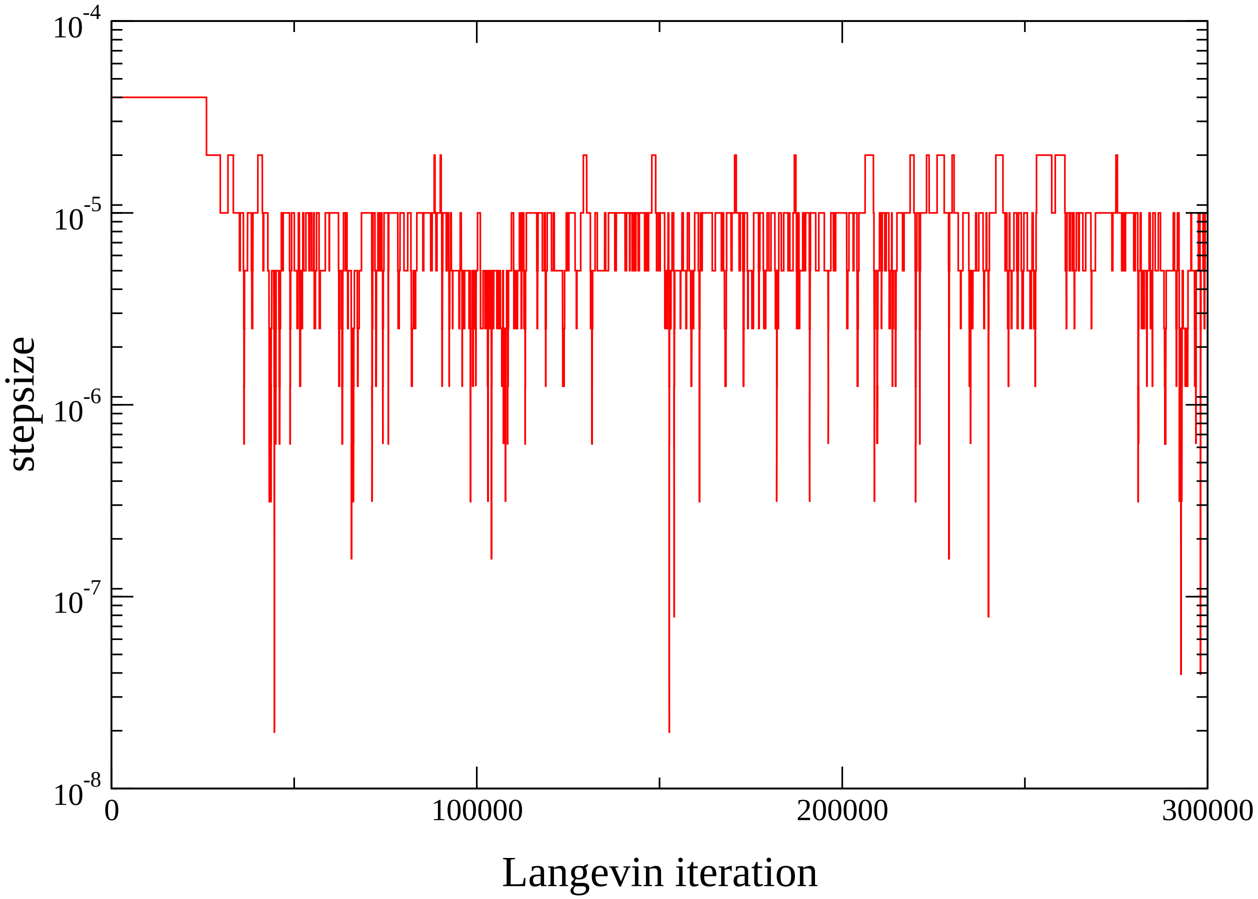
3. convergence to wrong limit

   $\Rightarrow$ better understood but not yet resolved

   `in progress`

Instabilities: heavy dense QCD

adaptive time step during the evolution



occasionally *very* small stepsize required
can go to longer Langevin times without problems

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 11

- 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

contrast with 3D XY model GA & James 10

SU(3) spin model

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

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

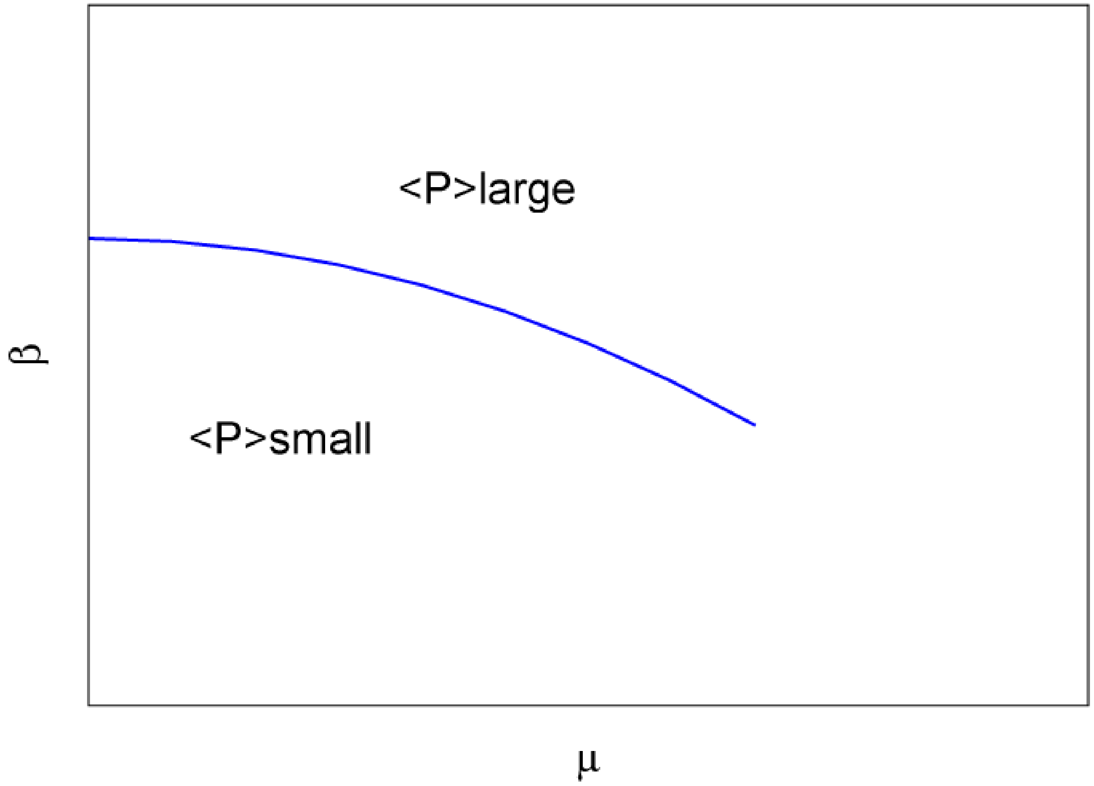
$$S_F = -h \sum_x \left[e^{\mu} P_x + e^{-\mu} P_x^* \right]$$

- 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

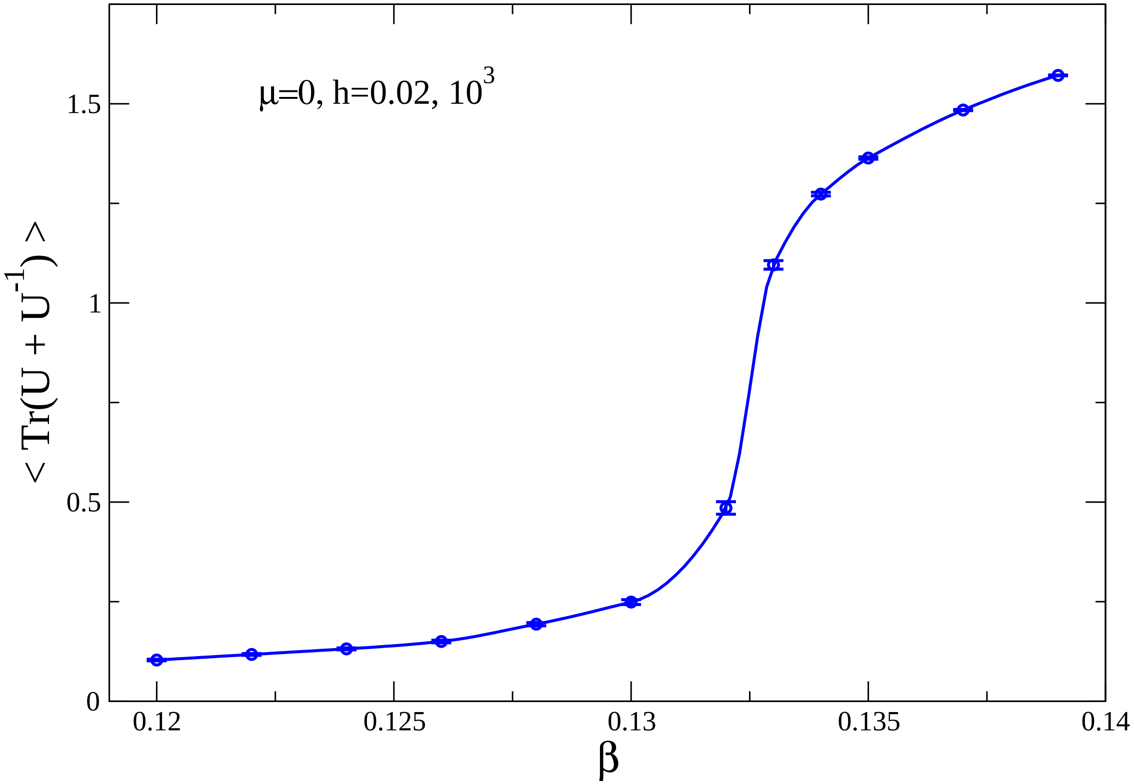
- phase structure



- effective model for QCD with static quarks

SU(3) spin model

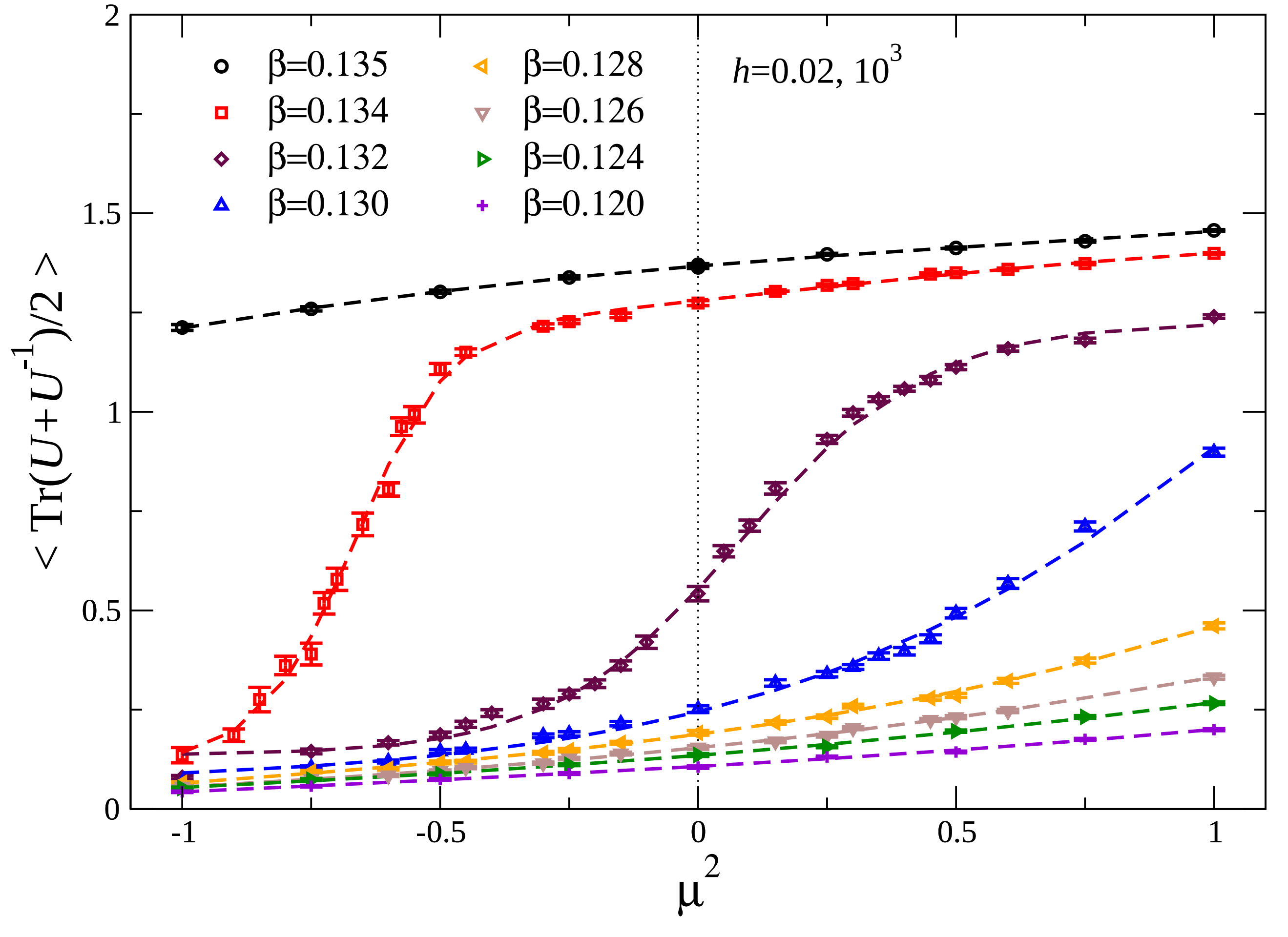
- phase structure at $\mu = 0$: $\langle P + P^* \rangle / 2$



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

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

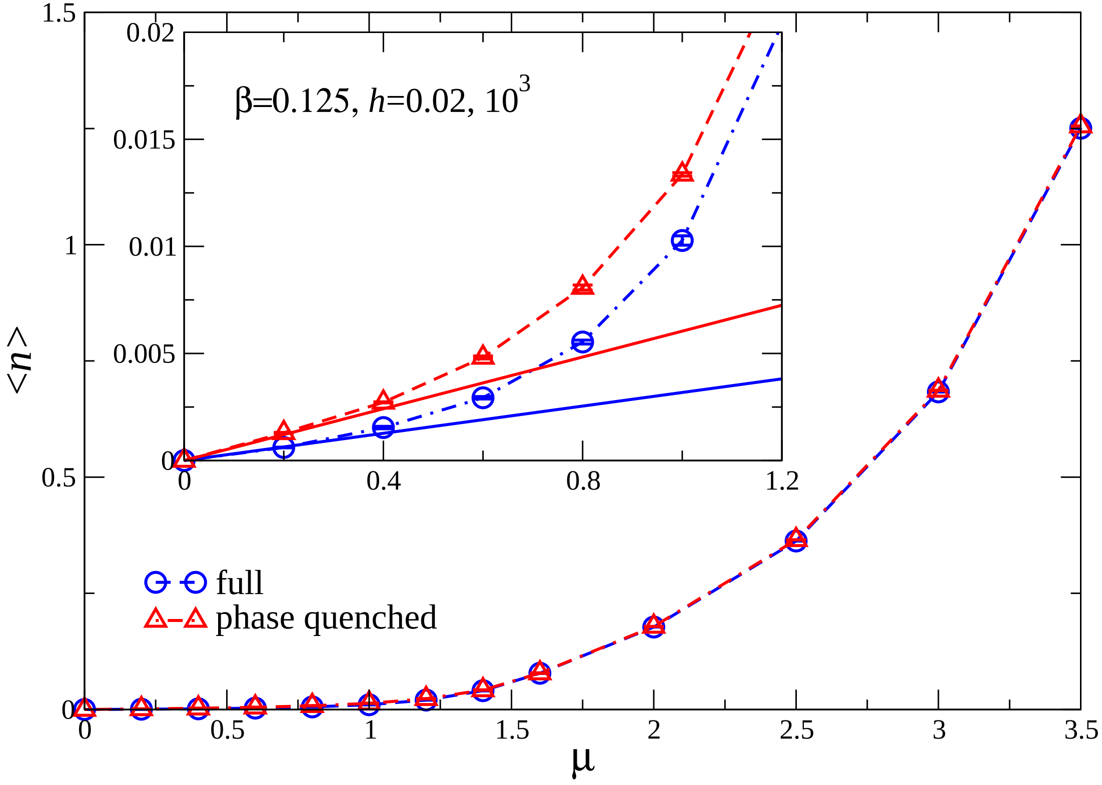
in terms of

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

c_2 is absent in phase-quenched theory

SU(3) spin model

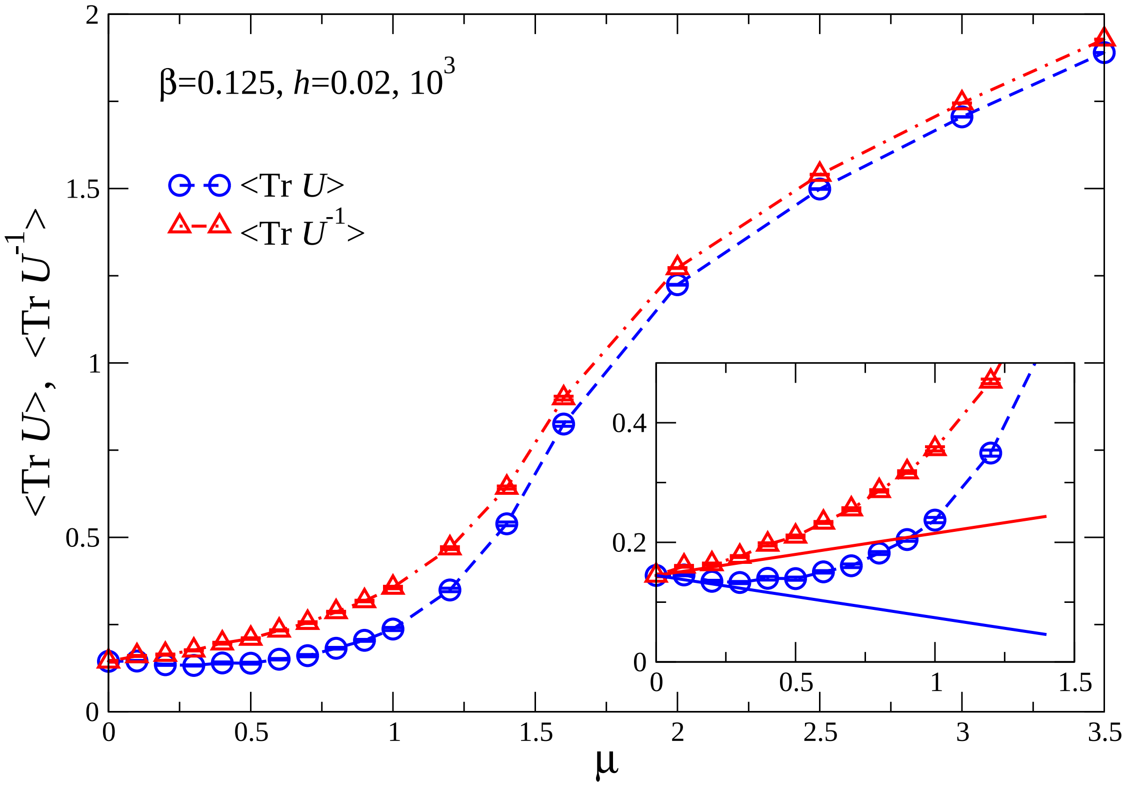
- start in 'confining' phase and increase μ
- density $\langle n \rangle = \langle h e^{\mu} P_x - h e^{-\mu} P_x^* \rangle$: no Silver Blaze region



- inset: lines from first-order Taylor expansion

SU(3) spin model

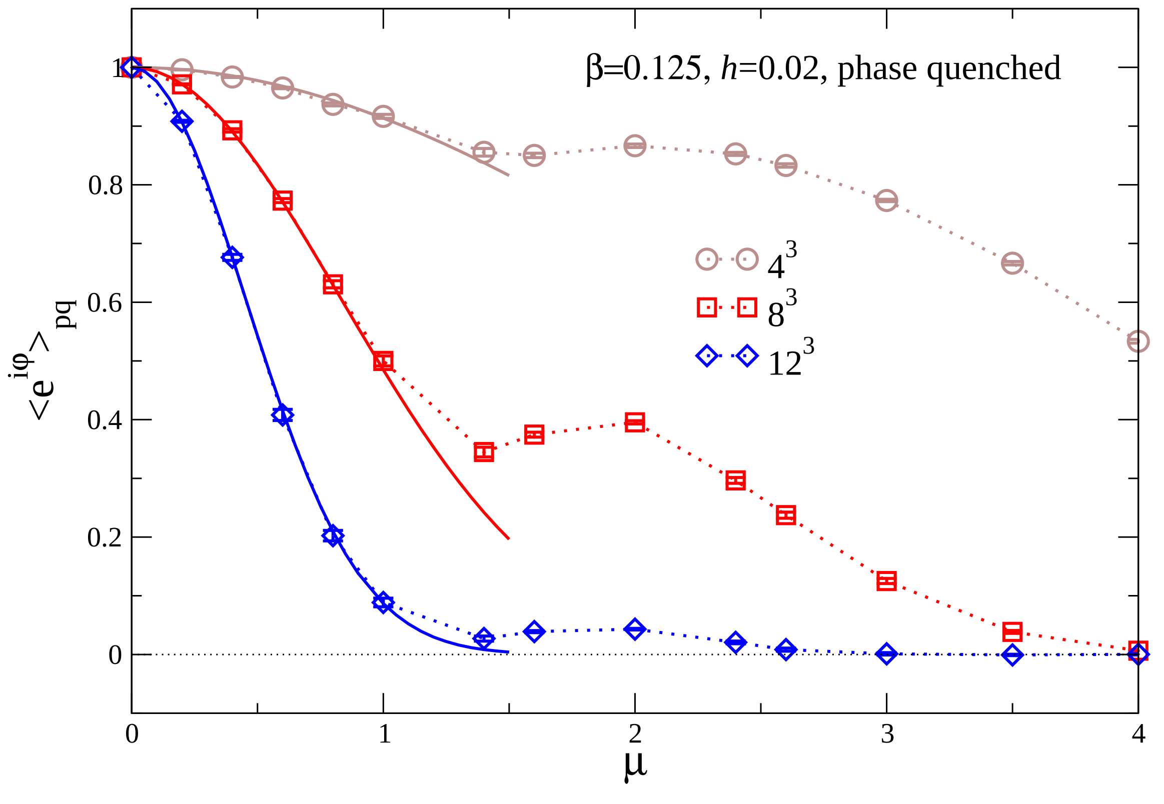
- start in 'confining' phase and increase μ
- splitting between $\langle P \rangle$ and $\langle P^* \rangle$: no Silver Blaze region



- inset: lines from first-order Taylor expansion

SU(3) spin model

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



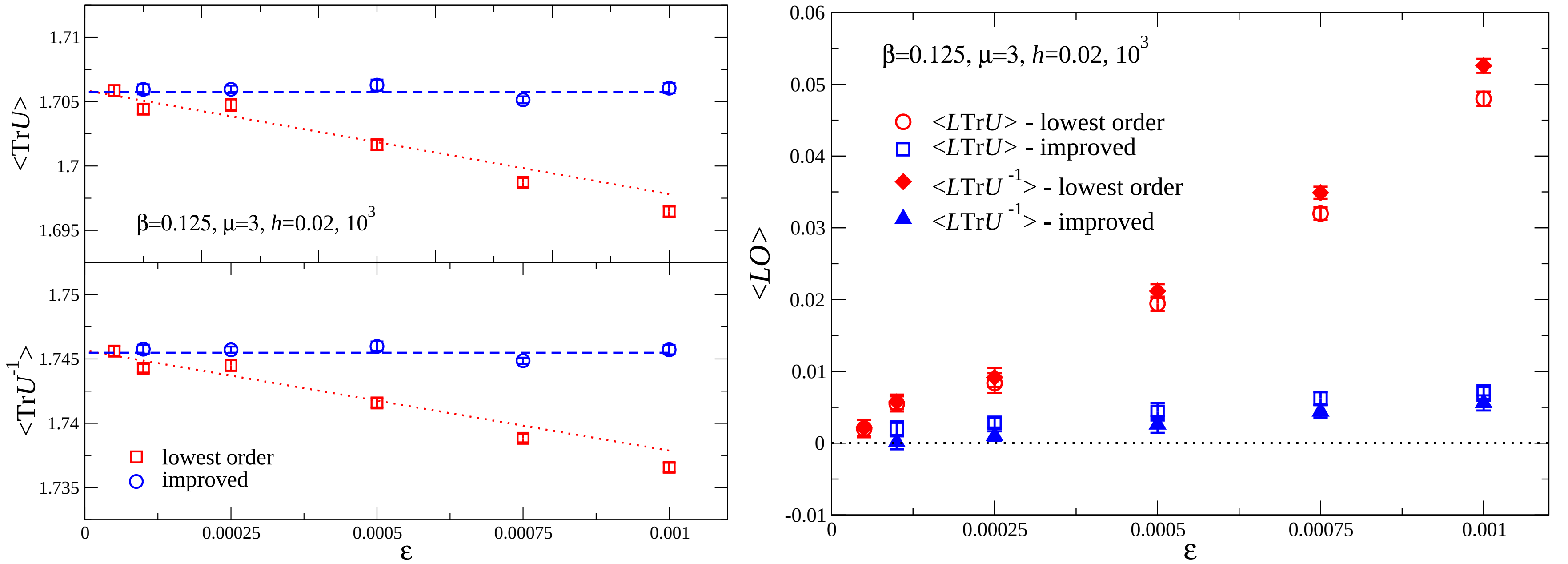
$$\Delta f \equiv f - f_{\mathrm{pq}} = -c_2 h^2 \mu^2 + \mathcal{O}(\mu^4) \qquad (c_2 < 0)$$

SU(3) spin model

beyond Taylor series: criteria for correctness $\langle LO \rangle = 0$

left: $\langle P \rangle$ (top) and $\langle P^* \rangle$ (bottom) at $\mu = 3$

right: criteria for correctness $\langle LO \rangle = 0$



improved stepsize algorithm to eliminate linear dependence

criteria satisfied as stepsize $\epsilon \to 0$

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

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

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

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

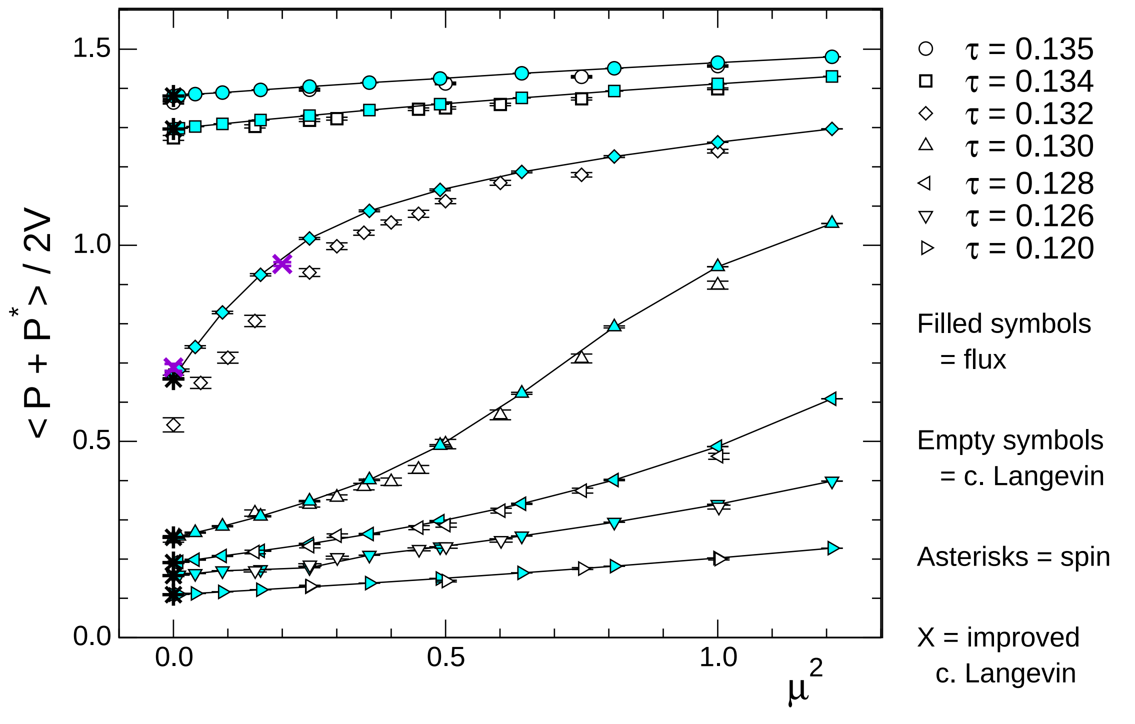
noise $\tilde{\alpha}_n = \frac{1}{2}\alpha_n + \frac{\sqrt{3}}{6}\xi_n \qquad \langle\alpha_n\alpha_{n'}\rangle = \langle\xi_n\xi_{n'}\rangle = 2\delta_{nn'}$

- 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

Success/failure

3D SU(3) spin model:

- complex Langevin passes all the tests: why?

3D XY model in the disordered phase:

- complex Langevin fails all the tests: why?

XY model

3D XY model [U(1) model] at nonzero μ

$$S = -\beta \sum_{x,\nu} \cos\left(\phi_x - \phi_{x+\hat{\nu}} - i\mu\delta_{\nu,0}\right)$$

$$= -\frac{1}{2}\beta \sum_{x,\nu} \left[e^{\mu\delta_{\nu,0}} U_x U^*_{x+\hat{\nu}} + e^{-\mu\delta_{\nu,0}} U^*_x U_{x+\hat{\nu}}\right]$$

- μ couples to the conserved Noether charge
- symmetry $S^*(\mu) = S(-\mu^*)$

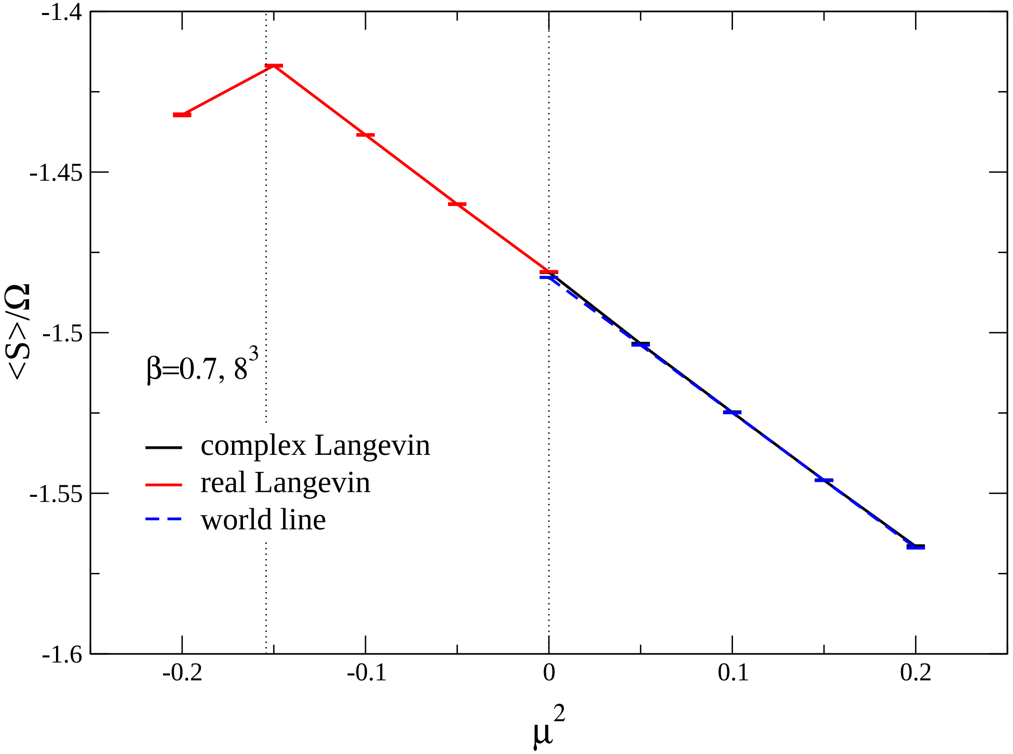
unexpectedly difficult to simulate with complex Langevin!

GA & James 10

- also studied by Banerjee & Chandrasekharan using worldline formulation hep-lat/1001.3648

Convergence: XY model

- comparison with known result (world line formulation)
- analytic continuation from imaginary $\mu = i\mu_{\rm I}$



action density versus μ^2

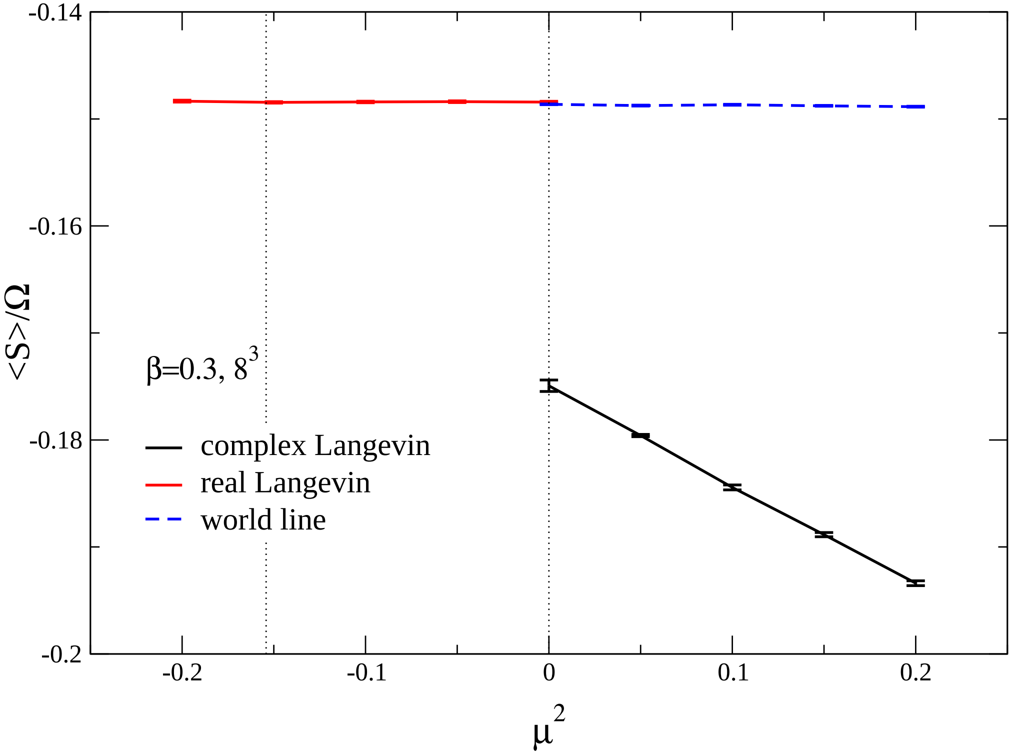
$\beta = 0.7$

ordered phase

- “Roberge-Weiss” transition at $\mu_{\rm I} = \pi/N_\tau$

Convergence: XY model

- comparison with known result (world line formulation)
- analytic continuation from imaginary $\mu = i\mu_{\rm I}$



action density versus μ^2

$\beta = 0.3$

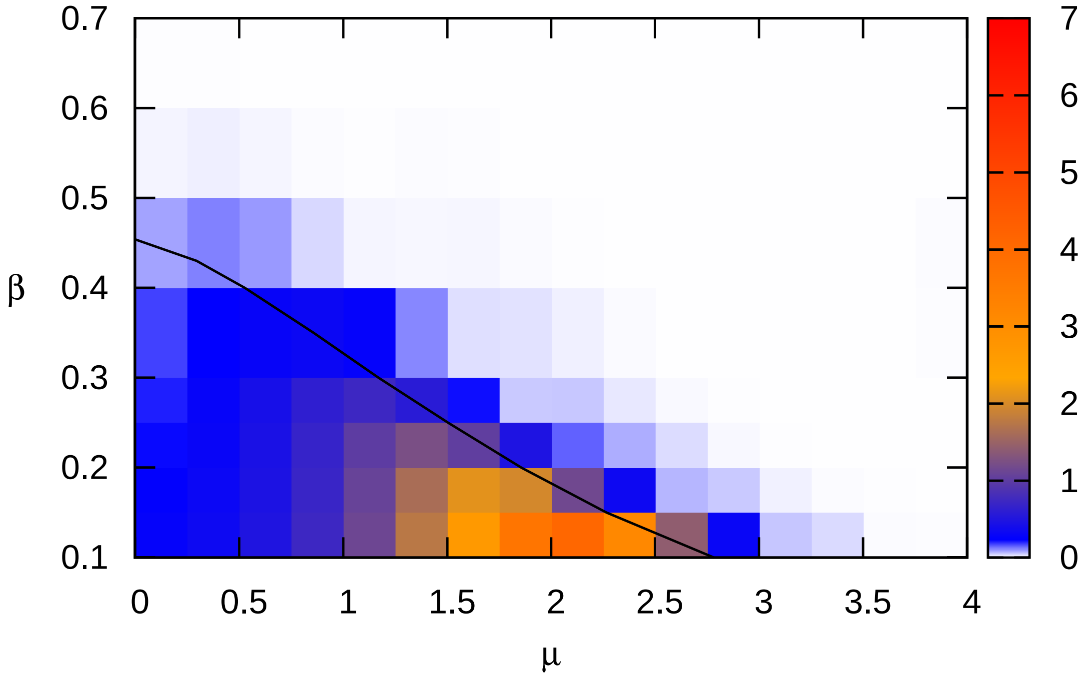
disordered phase

failure

Convergence: XY model

- comparison with known result (world line formulation)

phase diagram:



relative deviation:

$$\Delta S = \frac{\langle S \rangle_{\mathrm{cl}} - \langle S \rangle_{\mathrm{wl}}}{\langle S \rangle_{\mathrm{wl}}}$$

high β: ordered

low β: disordered

- phase boundary from Banerjee & Chandrasekharan
- highly correlated with ordered/disordered phase

Convergence: XY model

- apparent correct results in the ordered phase
- incorrect result in the disordered/transition region

diagnostics:

- distribution $P[\phi_{\rm R}, \phi_{\rm I}]$ qualitatively different
- classical force distribution qualitatively different

note:

- independent of strength of the sign problem

  failure not due to sign problem

U(1) versus SU(3)?

GA, FJ, ES, IOS, DS, in preparation

U(1) versus SU(N)

spin models: integrate over reduced Haar measure

- U(1): $U = e^{i\phi}$ $\int_{-\pi}^{\pi} d\phi$
- SU(N):

$U =$ diag $\left(e^{i\phi_1}, e^{i\phi_2}, \ldots, e^{i\phi_N}\right)$ $\phi_1 + \phi_2 + \ldots + \phi_N = 0$

$$\int_{-\pi}^{\pi} d\phi_1 \ldots d\phi_N \, \delta\left(\phi_1 + \phi_2 + \ldots + \phi_N\right) H(\{\phi_i\})$$

$$H(\{\phi_i\}) = \prod_{i<j} \sin^2\left(\frac{\phi_i - \phi_j}{2}\right)$$

role of Haar measure?

U(1) versus SU(N)

- study in effective one-link models:

$$S = -\beta \sum_{<xy>} \left[P_x P_y^* + P_x^* P_y\right] - h \sum_x \left[e^\mu P_x + e^{-\mu} P_x^*\right]$$

- nearest neighbours represent complex couplings

effective one-link model:

$$S = -\beta_1(\mu) P - \beta_2(\mu) P^*$$

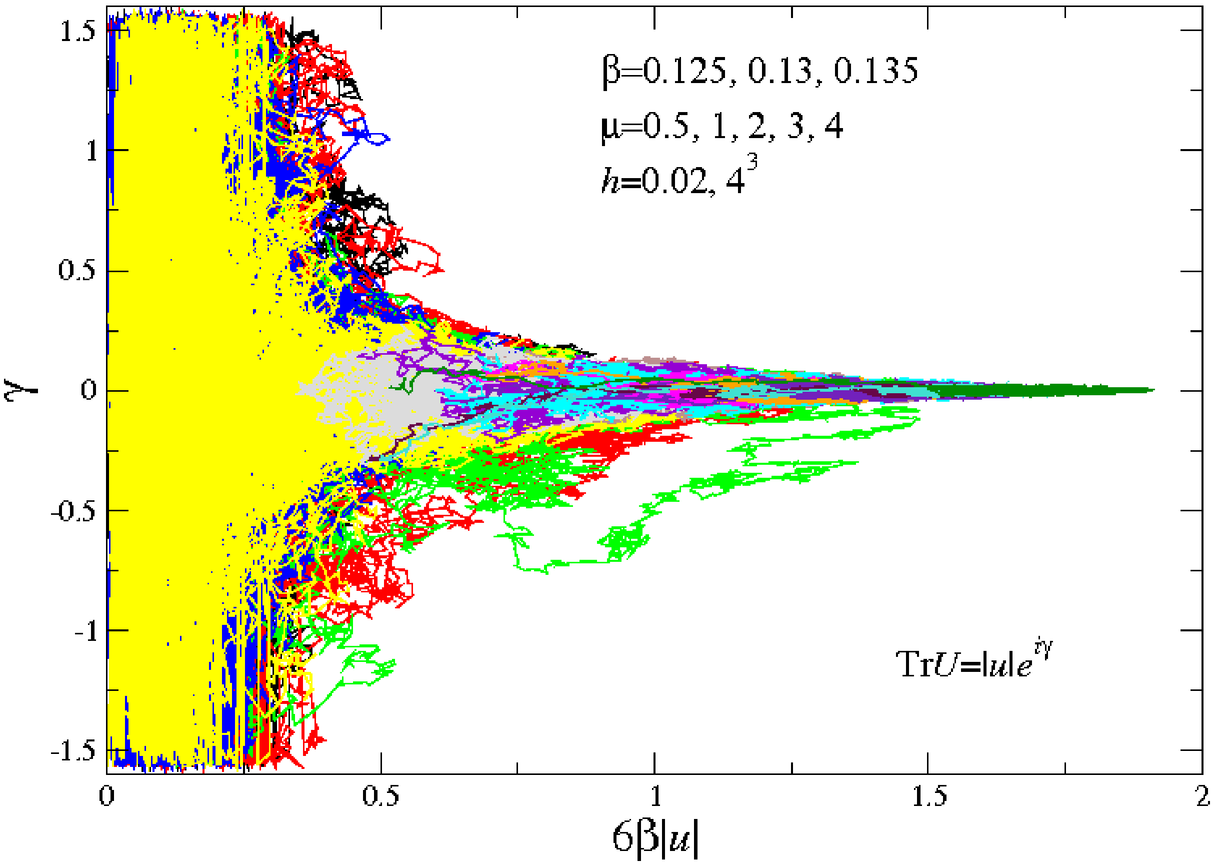
- complex couplings

$$\beta_1(\mu) = |\beta_{\rm eff}| e^{i\gamma} + h e^\mu \qquad\qquad \beta_2(\mu) = \beta_1^*(-\mu)$$

with $\beta_{\rm eff} = 6\beta P^*_{\pm\hat\nu} \in \mathbb{C}$

U(1) versus SU(N)

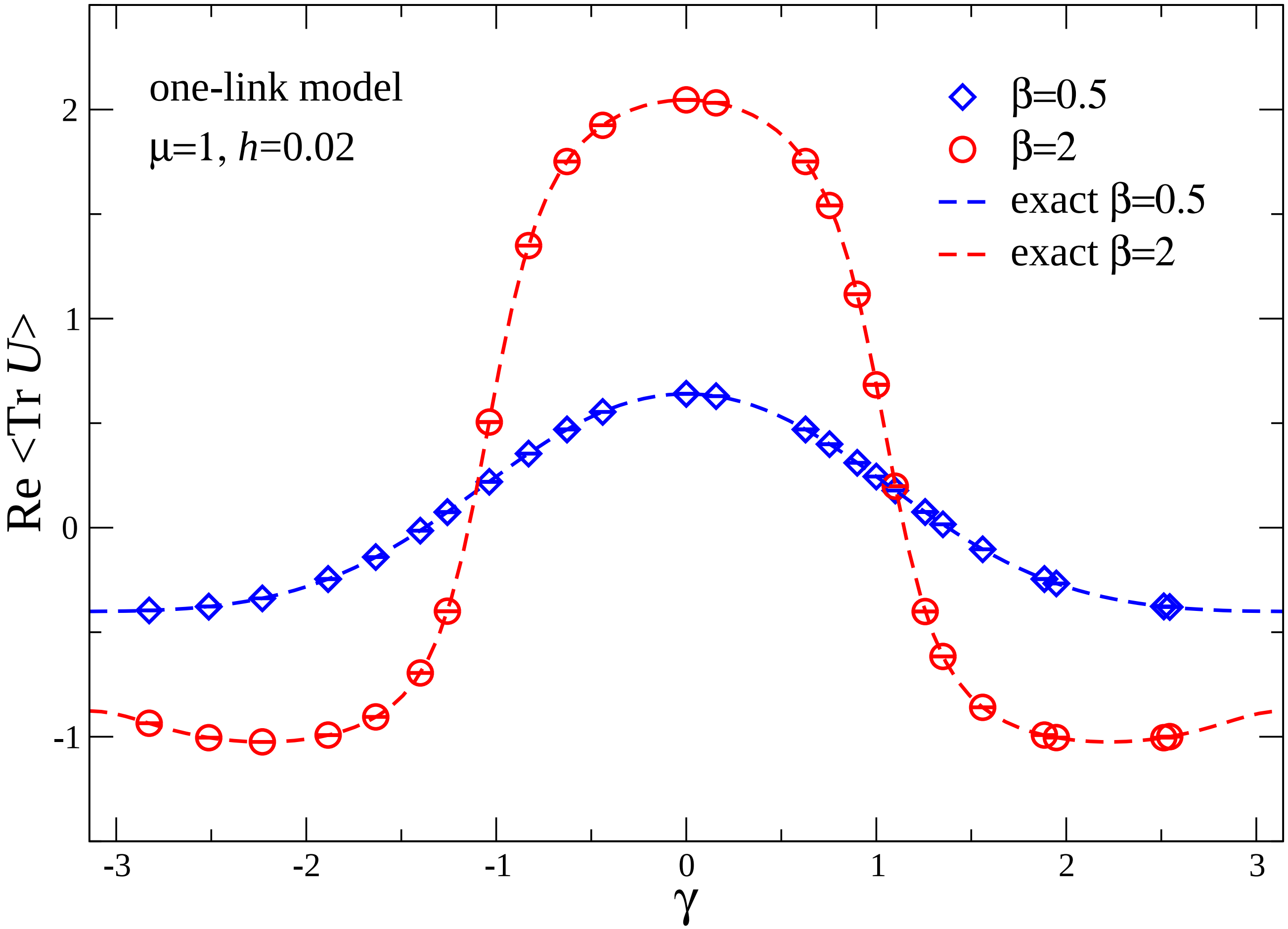
effective complex couplings: $\beta_{\rm eff} = 6\beta P^* = |\beta_{\rm eff}|e^{i\gamma} \in \mathbb{C}$



(preliminary)

U(1) versus SU(N)

SU(3) one-link model: $S = -\beta_1(\mu)P - \beta_2(\mu)P^*$



correct result for all angles γ

U(1) versus SU(N)

understanding: SU(2) one-link model

interpolate between U(1) and SU(N)

- one angle $\phi = x$ [SU(3) two angles, same conclusions]
- Haar measure $H(x) = \sin^2 x$
- partition function

$$Z = \int_{-\pi}^{\pi} dx\, H(x) e^{\beta \cos x}$$

- effective action

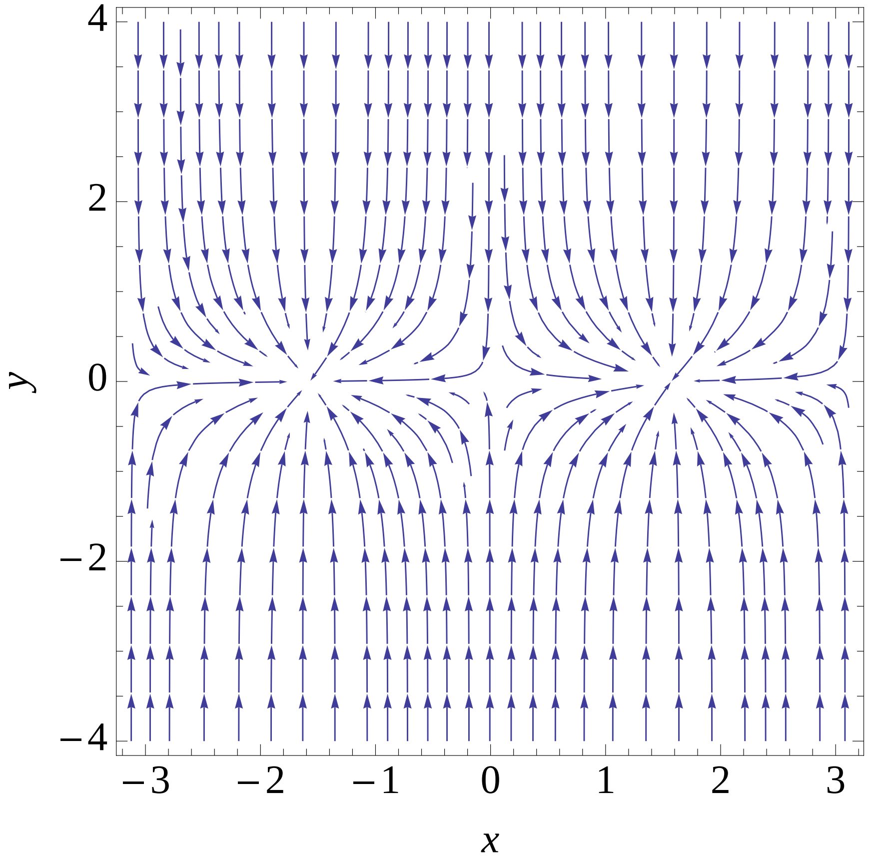
$$S = -\beta \cos x - 2d \ln \sin x \qquad \beta \in \mathbb{C}$$

- $d = 1$: SU(2) $d = 0$: U(1)

Flow: U(1) versus SU(N)

Haar measure only ($\beta = 0, d = 1$)

- singular at origin, use adaptive stepsize



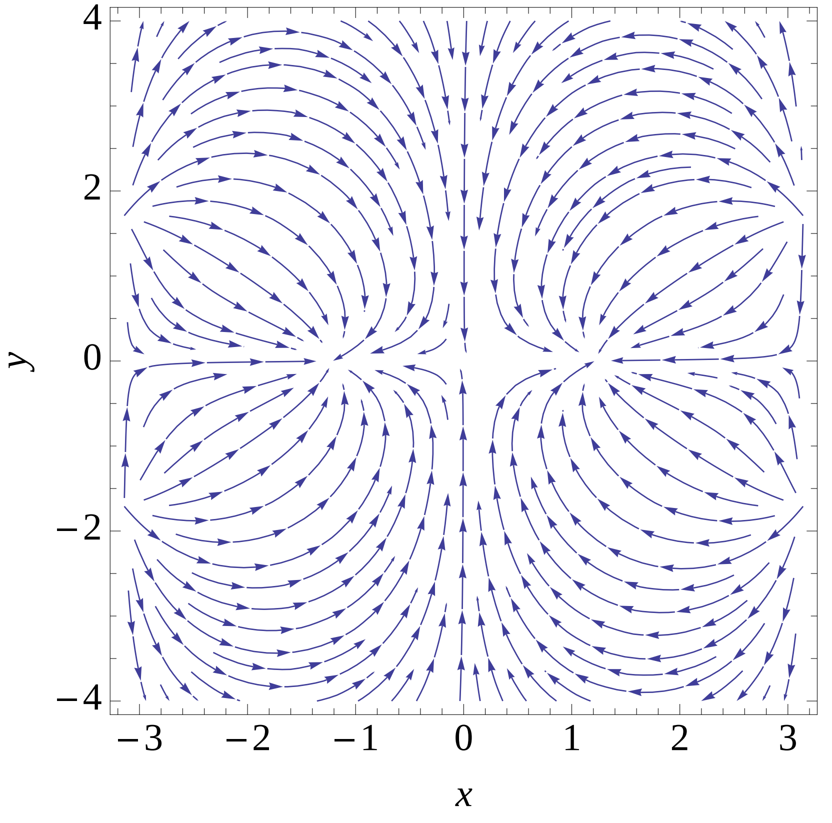
- always restoring! dynamics attracted to real manifold

Flow: U(1) versus SU(N)

$\beta \neq 0$: small imaginary fluctuations

- linear stability

$$\dot{y} = -\lambda y \qquad \lambda = \beta \cos x + \frac{2d}{1 - \cos 2x}$$



- real manifold linearly stable if $\beta < 2d$ (even marginally better)

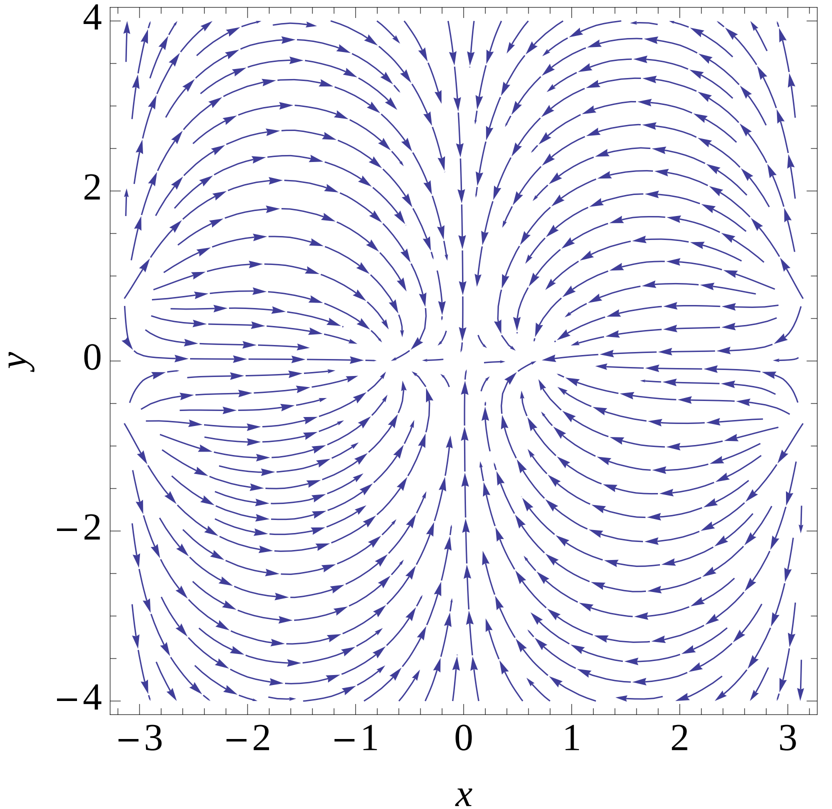
SU(2): $\beta = 0.4, d = 1$

Flow: U(1) versus SU(N)

$\beta \neq 0$: small imaginary fluctuations

- linear stability

$$\dot{y} = -\lambda y \qquad \lambda = \beta \cos x + \frac{2d}{1 - \cos 2x}$$



- real manifold linearly stable if $\beta < 2d$ (even marginally better)

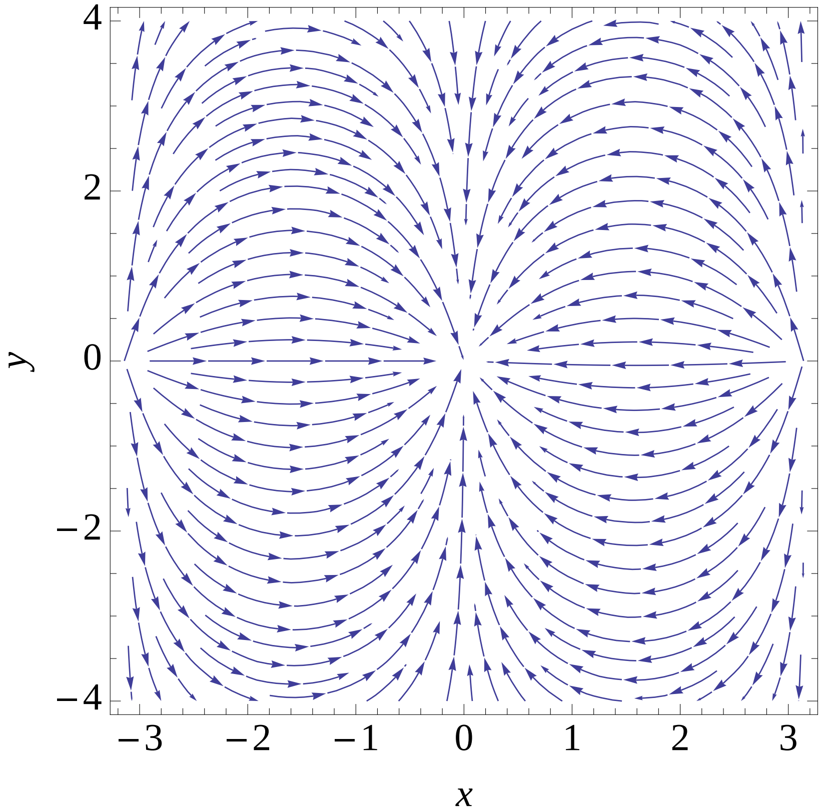
SU(2): $\beta = 2, d = 1$

Flow: U(1) versus SU(N)

$\beta \neq 0$: small imaginary fluctuations U(1)

- linear stability

$$\dot{y} = -\lambda y \qquad \lambda = \beta \cos x + \frac{2d}{1 - \cos 2x}$$



- real manifold linearly stable if $\beta < 2d$
- U(1): trivial Haar measure
- real manifold unstable!

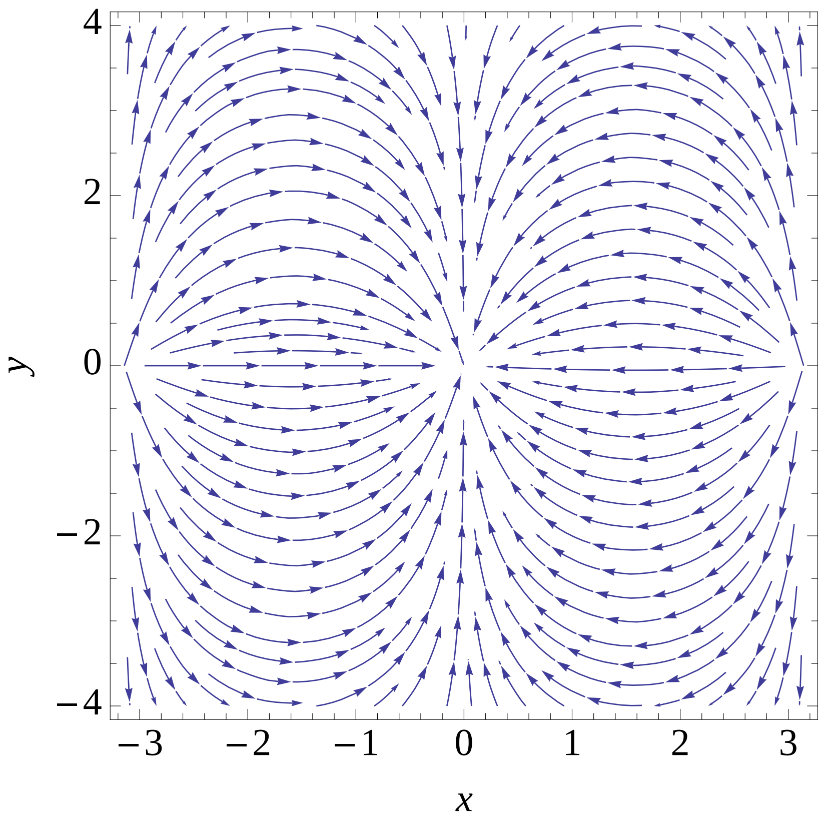
U(1): $\beta = 0.4, d = 0$

Flow: U(1) versus SU(N)

$\beta \neq 0$: small imaginary fluctuations U(1)

- linear stability

$$\dot{y} = -\lambda y \qquad \lambda = \beta \cos x + \frac{2d}{1 - \cos 2x}$$



- real manifold linearly stable if $\beta < 2d$
- U(1): trivial Haar measure
- real manifold unstable!

U(1): $\beta = 2, d = 0$

U(1) versus SU(N)

role of Haar measure in SU(N)

- dynamics due to Haar measure drives towards real manifold: attractive
- stable against small complex fluctuations

U(1)/XY model

- real manifold *unstable* against small complex fluctuations
- simulations at $\mu \to 0$ and $\mu = 0$ do not agree
- indeed observed in disordered phase of 3D XY model

  in ordered phase, nearest neighbours are correlated and one-link model is not applicable

  XY model becomes effectively Gaussian in ordered phase

Stabilizing drift

- Haar measure contribution to complex drift restoring
- controlled exploration of the complex field space

employ this: generate Jacobian by field redefinition

$$Z = \int dx\, e^{-S(x)} \qquad x = x(u) \qquad J(u) = \frac{\partial x(u)}{\partial u}$$

$$= \int du\, e^{-S_{\text{eff}}(u)} \qquad S_{\text{eff}}(u) = S(u) - \ln J(u)$$

drift: $K(u) = -S'_{\text{eff}}(u) = -S'(u) + J'(u)/J(u)$

which field redefinition?

singular at $J(u) = 0$ but restoring in complex plane

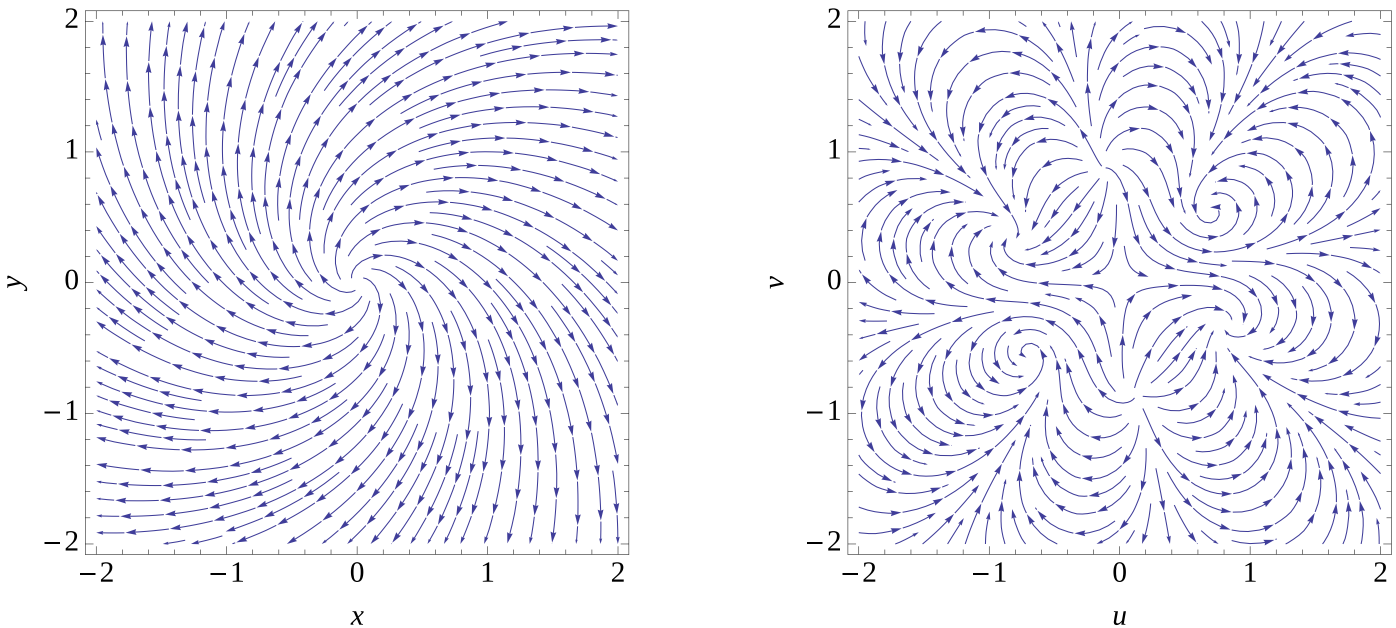
with Jan Pawlowski & FJ, ES, IOS, DS

Fun with complex Langevin

Gaussian example: defined when $\mathrm{Re}(\sigma) = a > 0$

$$Z = \int_{-\infty}^{\infty} dx\, e^{-\frac{1}{2}\sigma x^2} \qquad \sigma = a + ib \qquad \langle x^2 \rangle = \frac{1}{\sigma}$$

what if $a < 0$? flow in complex space for $a = -1, b = 1$:

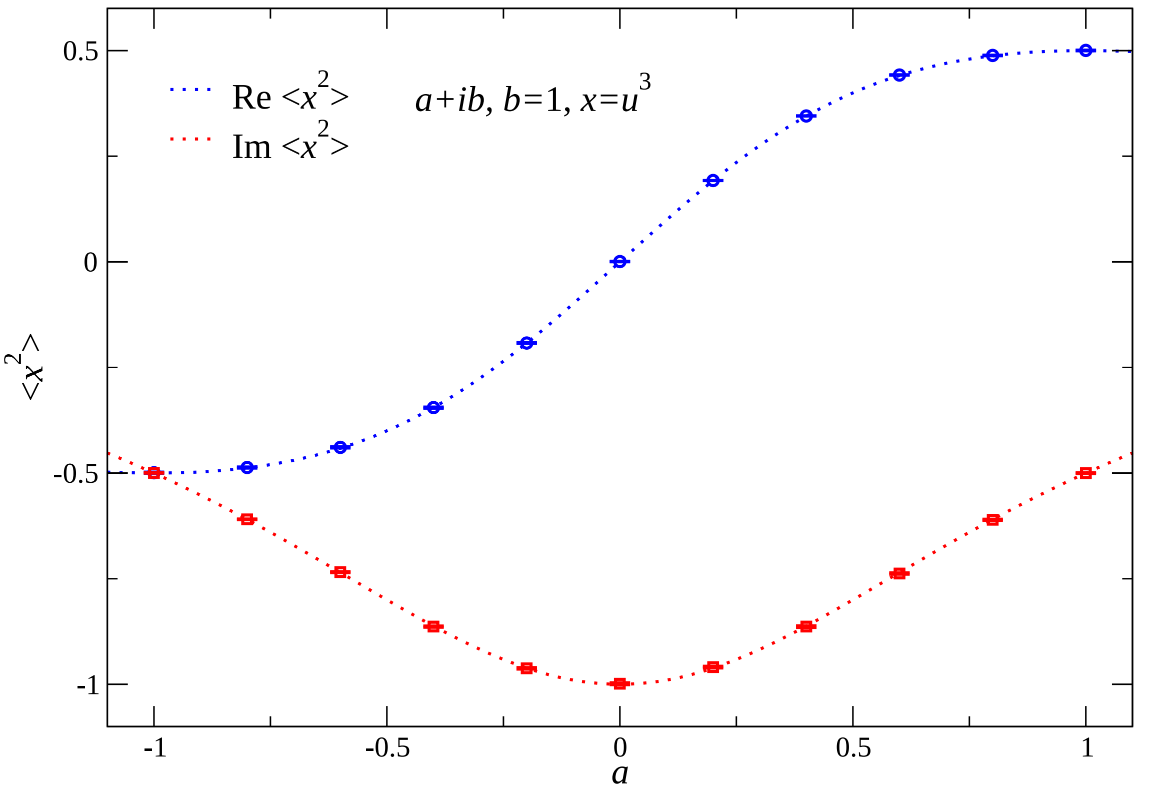


left: highly unstable

right: after transformation $x(u) = u^3$
attractive fixed points

Fun with complex Langevin

do CLE in the u formulation and compute $\langle x^2 \rangle = \langle u^6 \rangle$



$$\langle x^2 \rangle = \frac{1}{\sigma} = \frac{a - ib}{a^2 + b^2}$$

take also negative a

CLE finds the analytically continued answer to negative a!

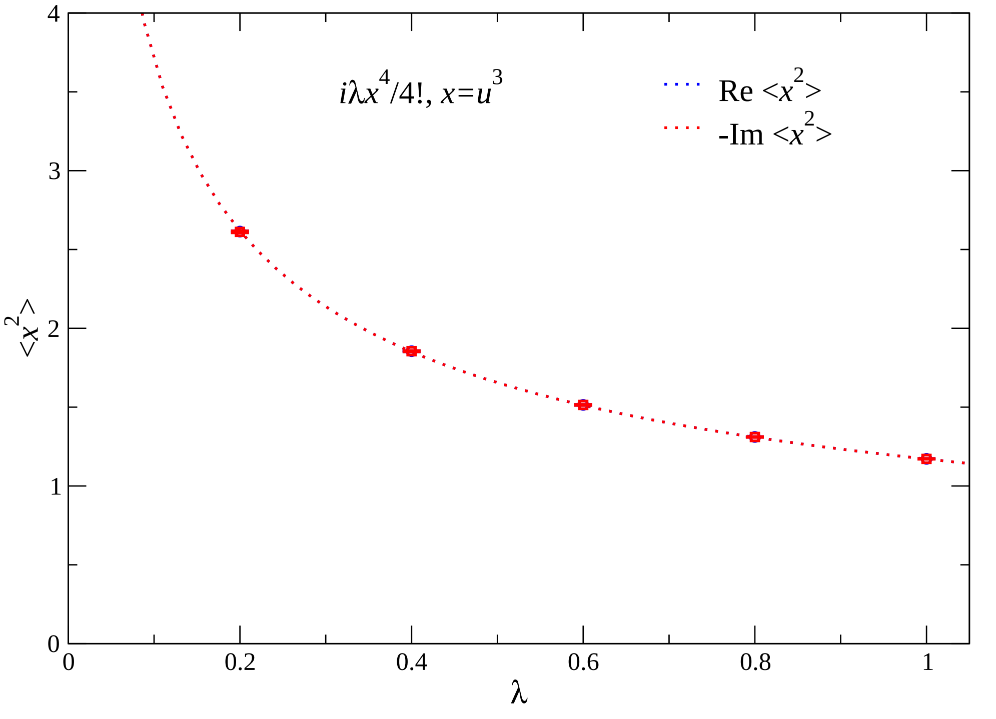
Fun with complex Langevin

quartic 'Minkowski' integral

$$Z = \int_{-\infty}^{\infty} dx \, \exp\left(-\frac{i\lambda}{4!}x^4\right)$$

correlator (defined via analytical continuation ($\lambda \to i\lambda$)

$$\langle x^2 \rangle = \frac{2\sqrt{3}}{\sqrt{\lambda}} \frac{\Gamma(\frac{3}{4})}{\Gamma(\frac{1}{4})}(1-i).$$



same transformation
$x(u) = u^3$

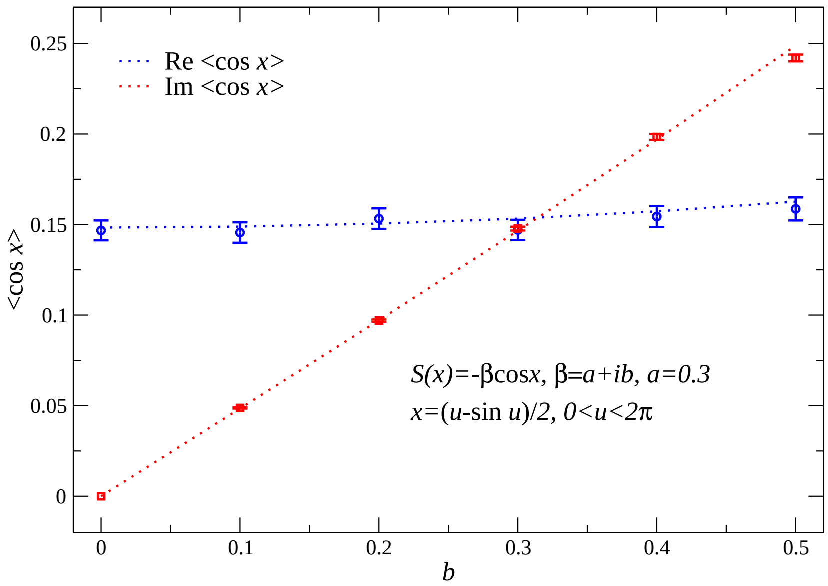
CLE finds correct answer!

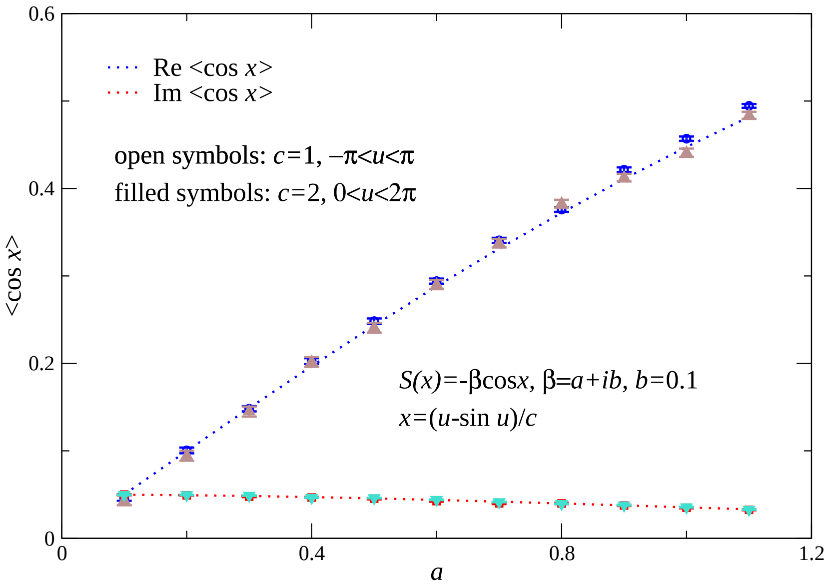
Fun with complex Langevin

towards XY model $Z = \int_{-\pi}^{\pi} dx\, e^{\beta \cos x}$ $\beta \in \mathbb{C}$

- transformation 1: $u = \cos x$, no ... real axis never stable!
- transformation 2: generate jacobian as in SU(2)

$$x = \frac{1}{c}(u - \sin u) \qquad J(u) = \frac{\partial x}{\partial u} = \frac{2}{c}\sin^2\frac{u}{2}$$





Fun with complex Langevin

towards XY model

- better effective one-link model

$$Z = \int_{-\pi}^{\pi} dx\, e^{\beta_1 \cos x + \beta_2 \sin x} \qquad \beta_{1,2} \in \mathbb{C}$$

- classical flow diagrams very turbulent
- no fun yet ...

implementation in 3D XY model hints that the idea is correct

optimal field redefinition not yet found

Summary

complex Langevin can handle

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

problems from the 80s:

- instabilities and runaways $\rightarrow$ adaptive stepsize
- convergence: correct result not guaranteed

in progress:

- theoretical foundation, criteria for correctness
- exploit freedom under field redefinitions and non-uniqueness of CLE