How to climb Mount Everest: the sign problem at finite density

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QCD phase diagram

partition function, after integrating out the quarks,

$$Z = \int DU\, e^{-S_{\rm YM}} \det D$$

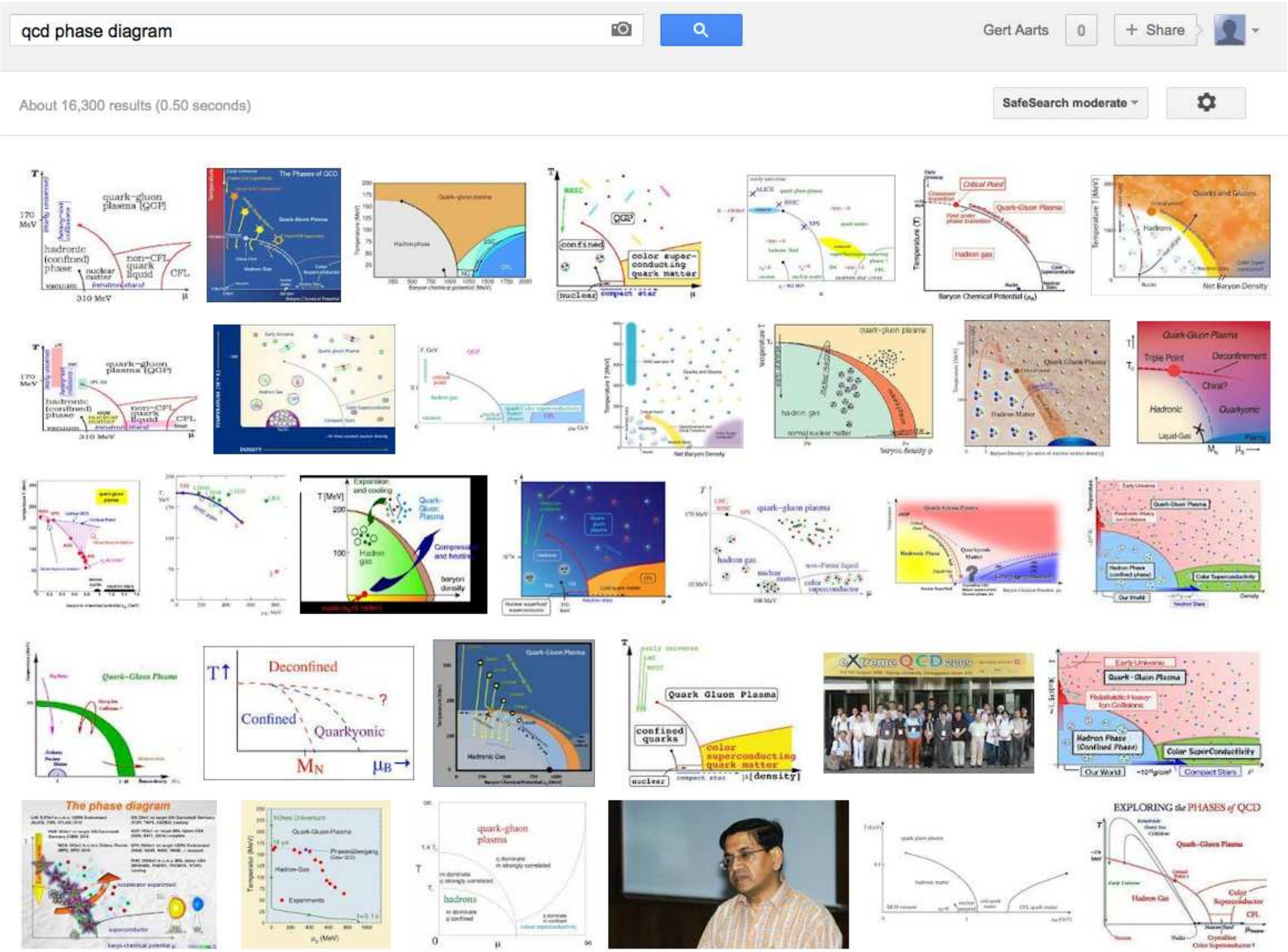
at nonzero quark chemical potential

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

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

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

Many QCD phase diagrams



Outline

- sign/overlap/Silver Blaze problems
- going complex ...
  - complex Langevin dynamics
  - distributions
  - SU(3) vs XY
  - stability of real manifold
- conclusion

Sign/overlap/Silver Blaze problems

integrate out the quarks: complex $\det D(\mu) = |\det D(\mu)|e^{i\theta}$

- sign problem due to complexity, not due to Grassmann nature: also appears in bosonic theories with $\mu \neq 0$
- ignore the phase: $|\det D(\mu)|$, phase quenching (pq)

Sign/overlap/Silver Blaze problems

integrate out the quarks: complex $\det D(\mu) = |\det D(\mu)|e^{i\theta}$

- **sign problem** due to complexity, not due to Grassmann nature: also appears in bosonic theories with $\mu \neq 0$
- ignore the phase: $|\det D(\mu)|$, phase quenching (pq)

if pq $\neq$ full, e.g. $\mu_{\rm pq}$(onset) $< \mu_{\rm full}$(onset)

- **overlap problem**: average sign

$$\langle e^{i\theta} \rangle_{\rm pq} = Z/Z_{\rm pq} = e^{-\Omega \Delta f} \qquad\qquad \Delta f = f - f_{\rm pq}$$

  vanishes exponentially with 4-volume Ω

- **Silver Blaze problem**: many cancelations to ensure that onset happens at the right critical μ Cohen 03

Sign/overlap/Silver Blaze problems

example: $N_f = 2$ QCD with $[\det D(\mu)]^2$

- phase-quenched: $|\det D(\mu)|^2 = \det D(\mu) \det D(-\mu)$
  $\Rightarrow$ isospin chemical potential

Sign/overlap/Silver Blaze problems

example: $N_f = 2$ QCD with $[\det D(\mu)]^2$

- phase-quenched: $|\det D(\mu)|^2 = \det D(\mu) \det D(-\mu)$
  $\Rightarrow$ isospin chemical potential

at $T = 0$:

- isospin: onset at $\mu = m_\pi/2$
  full: onset at $\mu \sim m_N/3$ (– binding energy)
- Silver Blaze region: $m_\pi/2 < \mu \lesssim m_N/3$
- intricate cancelations, e.g. eigenvalue density of Dirac operator is complex, highly oscillatory, with exp. large amplitude in thermodynamic limit
- precise integration to get correct cancelations

Osborn, Splittorff & Verbaarschot 05

Sign problem

Solving the sign problem $\sim$ *climbing Mount Everest*

`Philippe de Forcrand — Sign 2012, Regensburg`

Sign problem

Solving the sign problem $\sim$ *climbing Mount Everest*

Philippe de Forcrand – Sign 2012, Regensburg

- use standard approaches: may not get to the top
  (reweighting, small μ^2: Taylor series, analytical continuation, . . .)

Sign problem

Solving the sign problem $\sim$ *climbing Mount Everest*

Philippe de Forcrand – Sign 2012, Regensburg

- use standard approaches: may not get to the top
- solve related theories: may end up on the wrong top
  (two-color QCD, strong-coupling QCD, effective models, . . .)

Sign problem

Solving the sign problem $\sim$ *climbing Mount Everest*

Philippe de Forcrand — Sign 2012, Regensburg

- use standard approaches: may not get to the top
- solve related theories: may end up on the wrong top
- use complex Langevin dynamics: climb without any ropes or guidance ...

Sign problem

Solving the sign problem $\sim$ climbing Mount Everest

Philippe de Forcrand — Sign 2012, Regensburg

- use complex Langevin dynamics: climb without any ropes or guidance ...

starting point is below sea level!

Sign problem

Solving the sign problem $\sim$ climbing Mount Everest

Philippe de Forcrand – Sign 2012, Regensburg

- use complex Langevin dynamics: climb without any ropes or guidance ...

at least some height was tackled ....

Complex integrals

- consider simple integral

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

- complete the square/saddle point approximation:

  into complex plane

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

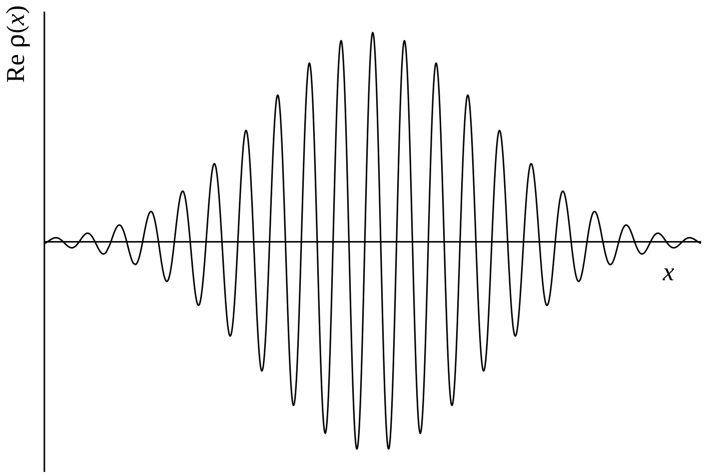
radically different approach:

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

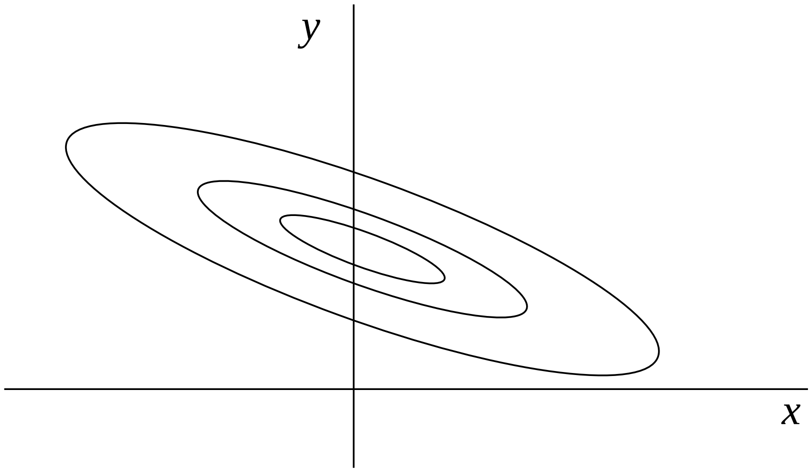
Complexified field space

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

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

why keep talking about it? recent examples in which CL

- can solve Silver Blaze problem
- can handle severe sign problems
- gives the correct result (!)
- analytical understanding improving

Complex Langevin dynamics

various scattered results since mid 1980s

here: review finite density results obtained with

Nucu Stamatescu, Erhard Seiler, Frank James
Denes Sexty, Jan Pawlowski, . . .

0807.1597 [GA & IOS] ... 1212.5231 [GA, FJ, JP, ES, DS & IOS]

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

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

- 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 $P(x, y; t)$

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

- 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 fields:

- (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($N, \mathbb{C}$)

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

  see e.g. GA, ES & IOS 0912.3360 Duncan & Niedermaier 1205.0307

- 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) 0912.3360, 1101.3270

- smooth connection with original distribution when $\mu \sim 0$?

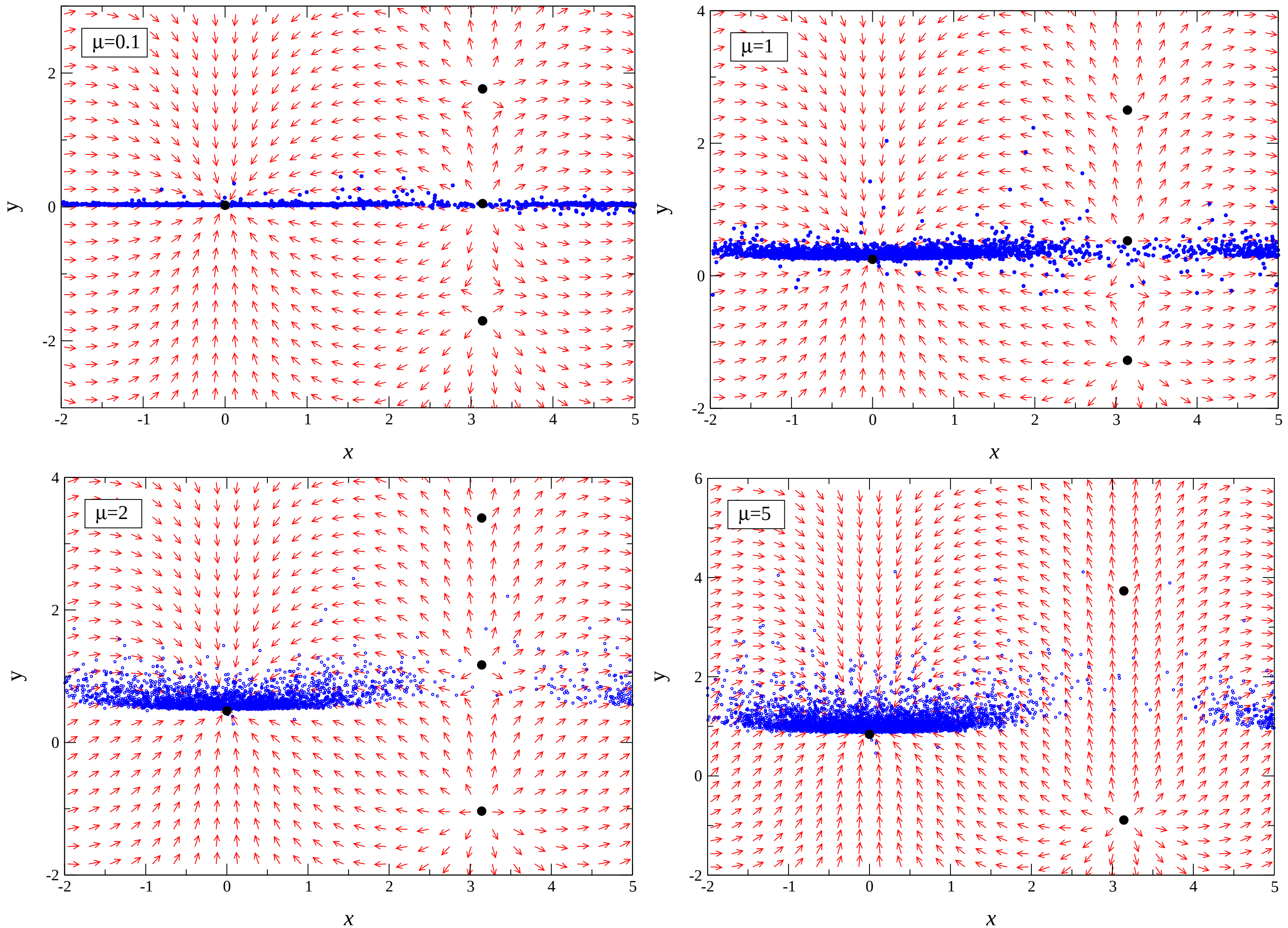
  GA, FJ, JP, ES, DS & IOS 1212.5231

study with histograms, scatter plots, flow

Distributions

distribution in well-behaved example

GA & IOS 0807.1597



SU(3) spin model vs XY model

contrast two three-dimensional spin models:

SU(3) and XY models GA & FJ 1005.3468, 1112.4655

- both can also be solved with worldline/flux methods
  Banerjee & Chandrasekharan 1001.3648
  Gattringer (& Mercado) 1104.2503, 1204.6074

SU(3) spin model:

- earlier solved with complex Langevin
  Karsch & Wyld 85 Bilic, Gausterer & Sanielevici 88
- effective Polyakov loop model for heavy quarks
- paradigm for strong-coupling/hopping expansions
  Philipsen, Langelage et al 09-12

SU(3) spin model

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

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

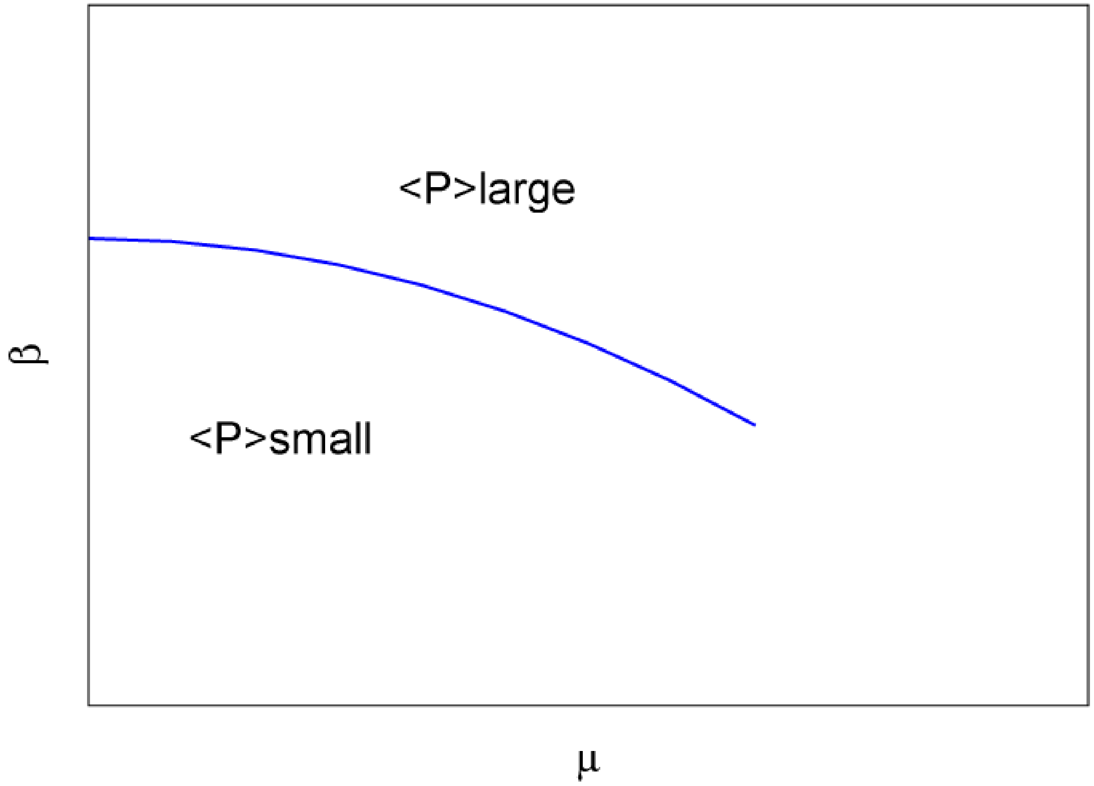
$$S_F = -h \sum_x \left[e^\mu P_x + e^{-\mu} P_x^* \right]$$

- SU(3) matrices: $P_x = \mathrm{Tr}\, U_x$, $P_x^* = \mathrm{Tr}\, U_x^\dagger = \mathrm{Tr}\, U_x^{-1}$
- gauge action: nearest neighbour Polyakov loops
- (static) quarks represented by Polyakov loops
- complex action $S^*(\mu) = S(-\mu^*)$

justification of complex Langevin:
out of many criteria: analyticity in μ^2, imag $\rightarrow$ real μ

SU(3) spin model

- phase structure

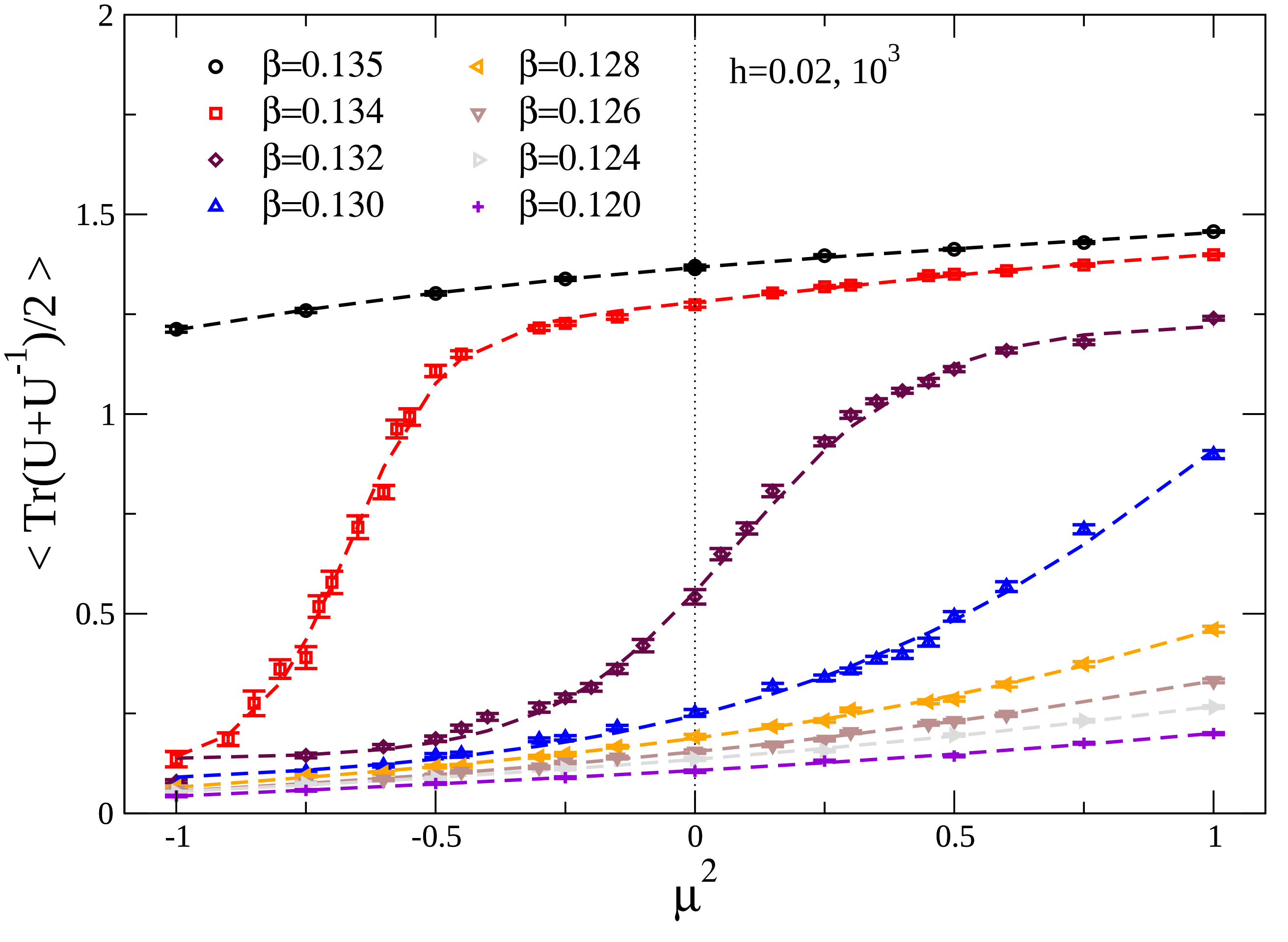


- effective model for QCD with static quarks

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

XY model

3D XY model [U(1) model] at nonzero μ

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

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

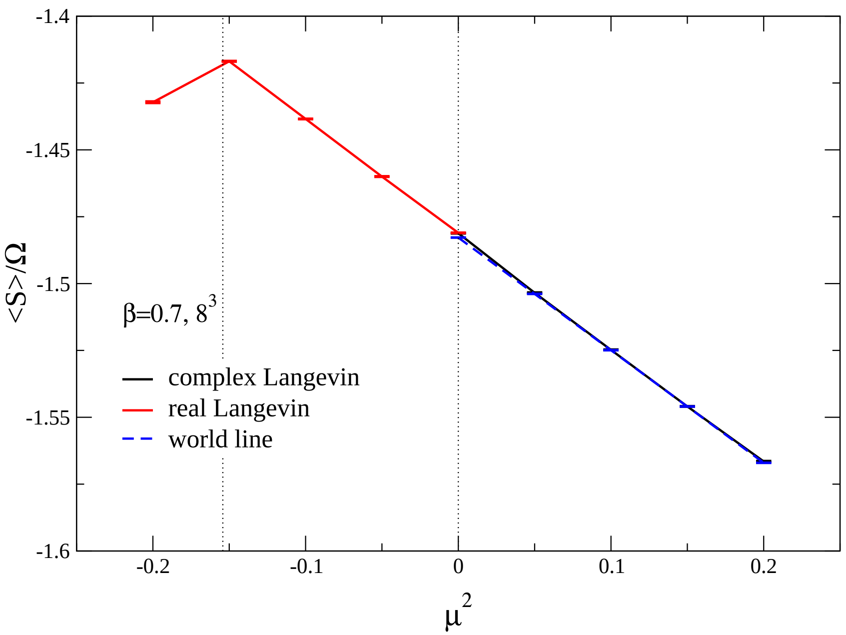
- μ couples to the conserved Noether charge
- symmetry $S^*(\mu) = S(-\mu^*)$

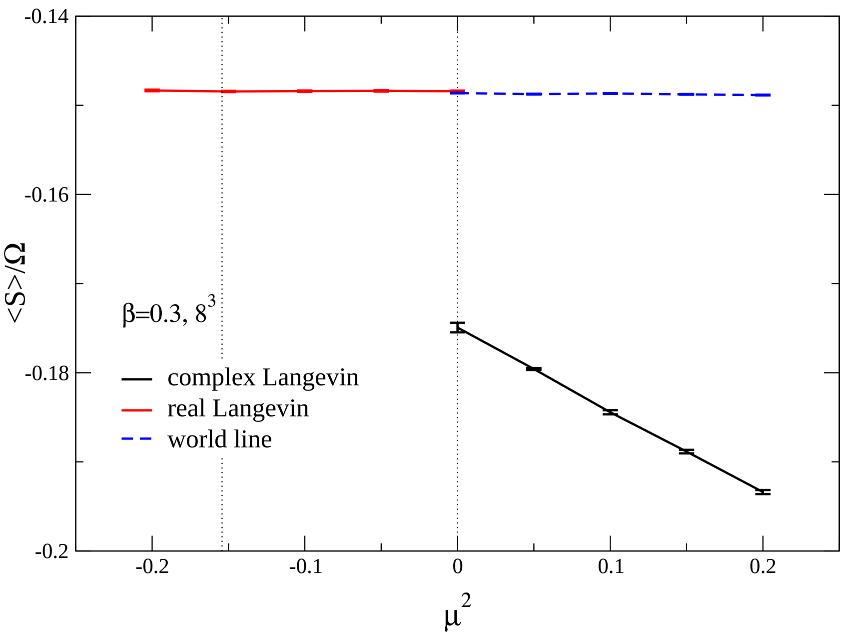
phase structure as in SU(3) model:

- disordered phase at small β, μ
- ordered phase at large β, μ

XY model

- analyticity in μ^2: action density around $\mu^2 \sim 0$





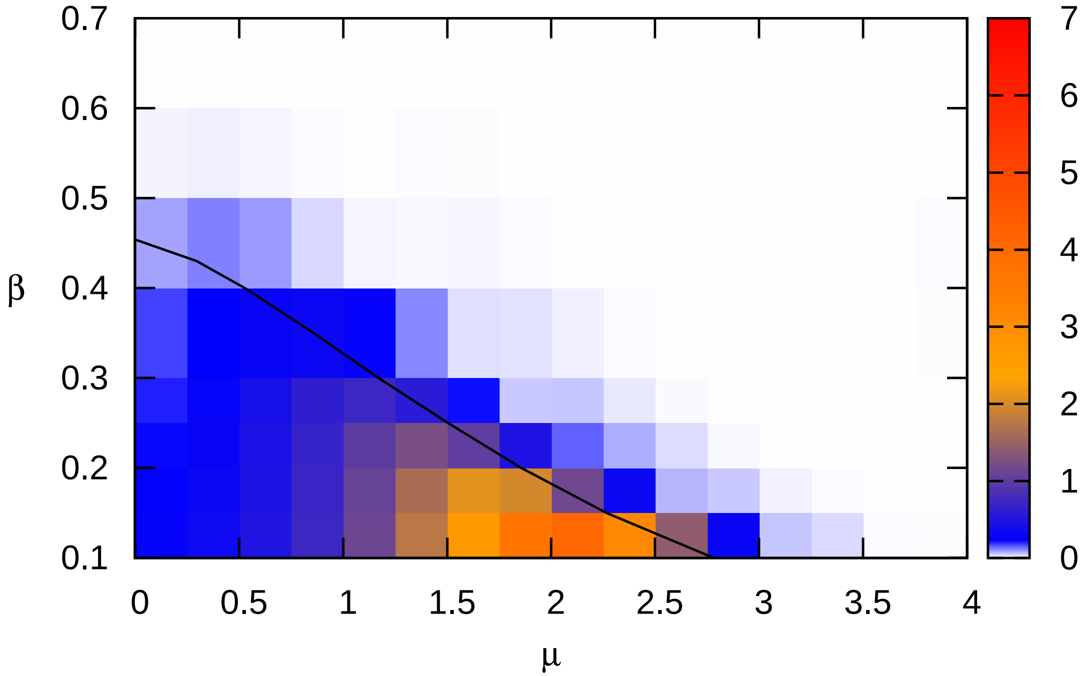
$\beta = 0.7$ ordered phase $\qquad$ $\beta = 0.3$ disordered phase

- failure in disordered phase: non-analytic
- aside: “Roberge-Weiss” transition at $\mu_{\rm I} = \pi / N_\tau$

XY model

- comparison with 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
- failure highly correlated with ordered/disordered phase

XY model

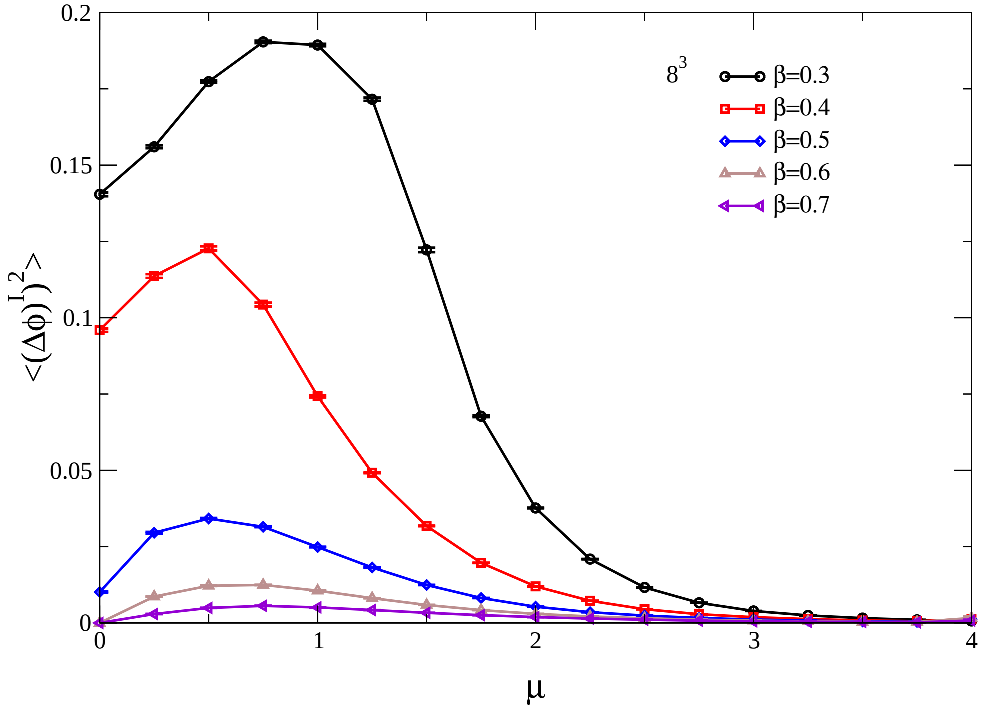
- incorrect result in the disordered/transition region

diagnostics:

width of distribution in $\phi_{\rm I}$ direction

$\langle(\Delta\phi_{\rm I})^2\rangle$

jumps discontinuously



- distribution $P[\phi_{\rm R}, \phi_{\rm I}]$ at $\mu \sim 0$ not smoothly connected to distribution $\rho[\phi]$ at $\mu = 0$
- aside: independent of strength of the sign problem

U(1) versus SU(N)

compare 3D spin models: reduce to effective one-link models

- example: SU(3)

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

- nearest neighbours represent complex couplings

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

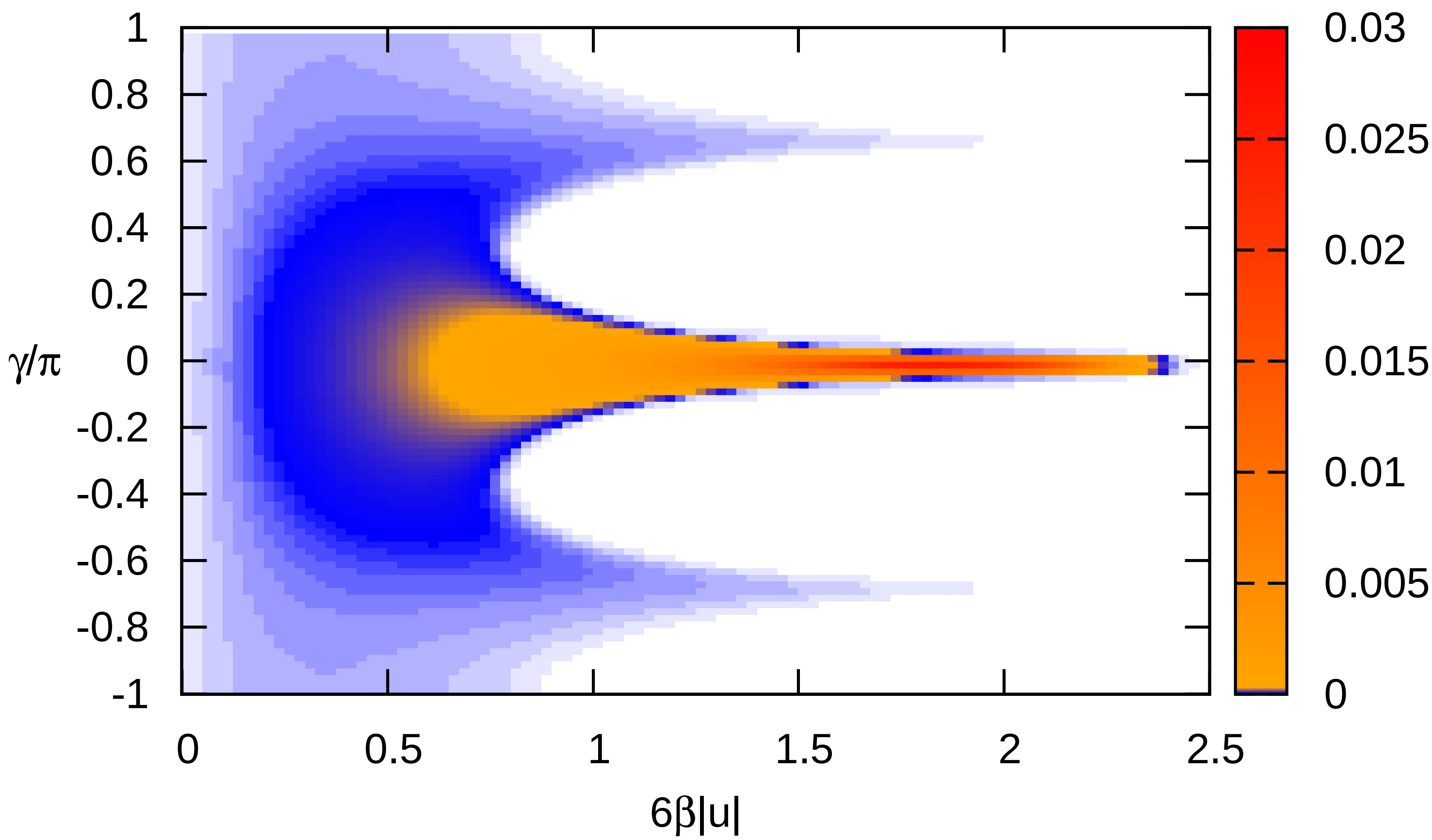
- complex couplings

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

with $\beta_{\text{eff}} = 6\beta P^*_{\pm\hat{\nu}} = 6\beta |u| e^{i\gamma} \in \mathbb{C}$

U(1) versus SU(N)

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



$\beta = 0.125, 0.13, 0.135 \qquad \mu = 0.5, 1, 2, 3, 4 \qquad h = 0.02 \qquad 12^3$

U(1) versus SU(N)

compare effective one-link models: integration over angles

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

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

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

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

role of reduced Haar measure?

U(1) versus SU(N)

compare U(1) and SU(2) one-link models

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

$$Z_{\mathrm{U}(1)} = \int_{-\pi}^{\pi} dx\, e^{\beta \cos x} \qquad Z_{\mathrm{SU}(2)} = \int_{-\pi}^{\pi} dx\, \sin^2 x\, e^{\beta \cos x}$$

- differ only in reduced Haar measure
- effective action

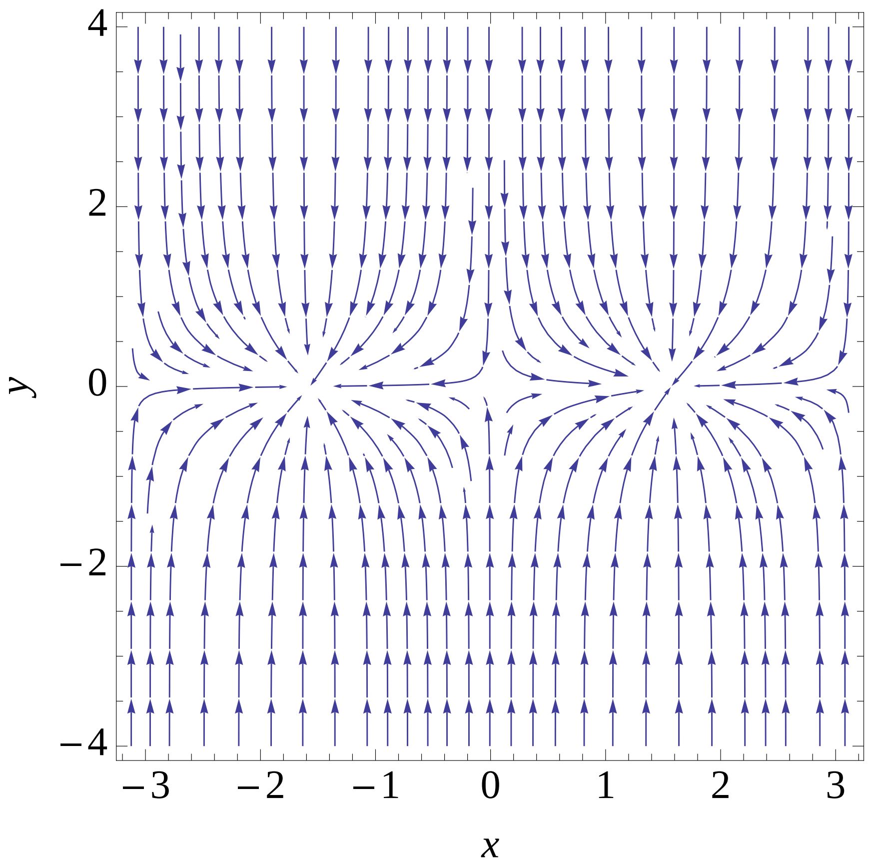
$$S = -\beta \cos x - 2d \ln \sin x \qquad \beta \in \mathbb{C}$$

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

Flow: U(1) versus SU(N)

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

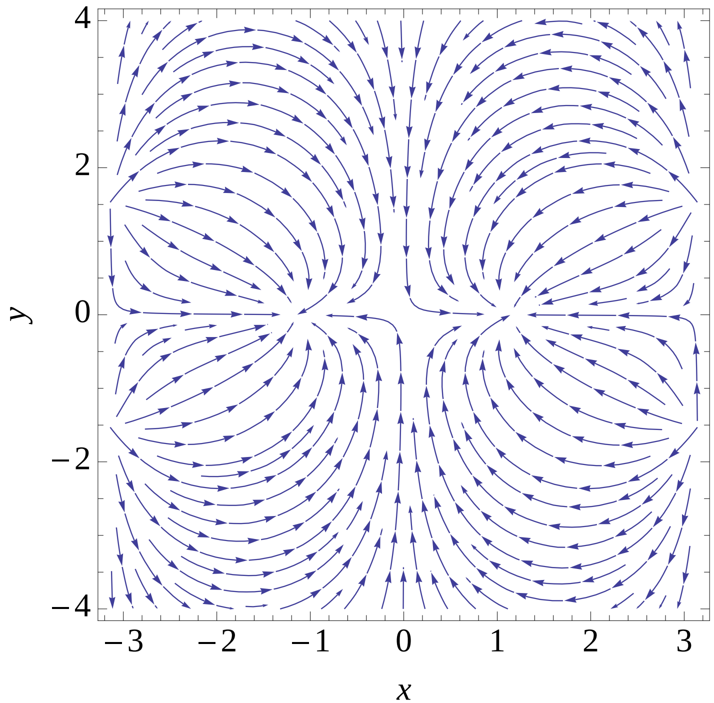
- singular at origin, use adaptive stepsize

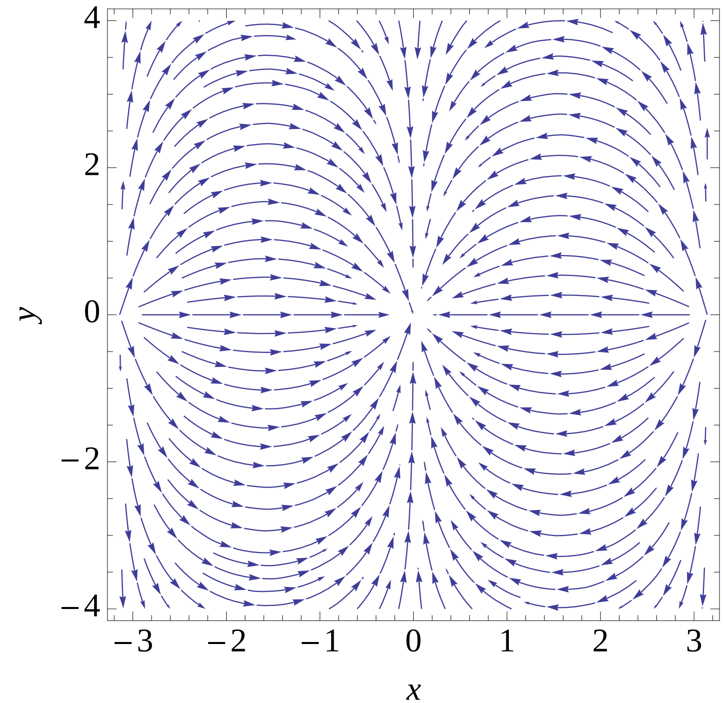


- always restoring! dynamics attracted to real manifold

Flow: U(1) versus SU(N)

$\beta \neq 0$: small imaginary fluctuations





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

- linear stability $\dot{y} = -\lambda y$ $\lambda = \beta \cos x + \frac{4d}{1 - \cos 2x}$
- SU(2): real manifold linearly stable if Re $\beta \lesssim 5.19$

U(1) versus SU(N)

role of reduced Haar measure in SU(N)

- dynamics due to reduced 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 is effectively Gaussian

Stabilizing drift

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

employ this: generate Jacobian by field redefinition

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

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

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

which field redefinition?

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

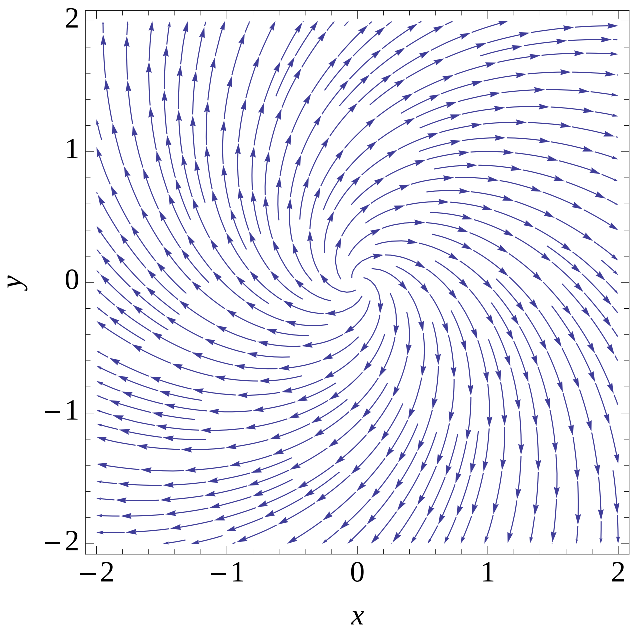
GA, FJ, JP, ES, DS & IOS 1212.5231

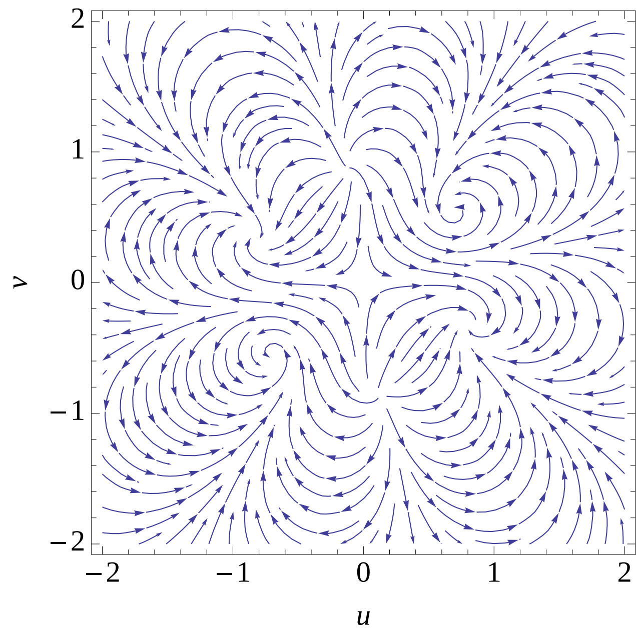
Field redefinitions: Gaussian

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 $a = -1, b = 1$:



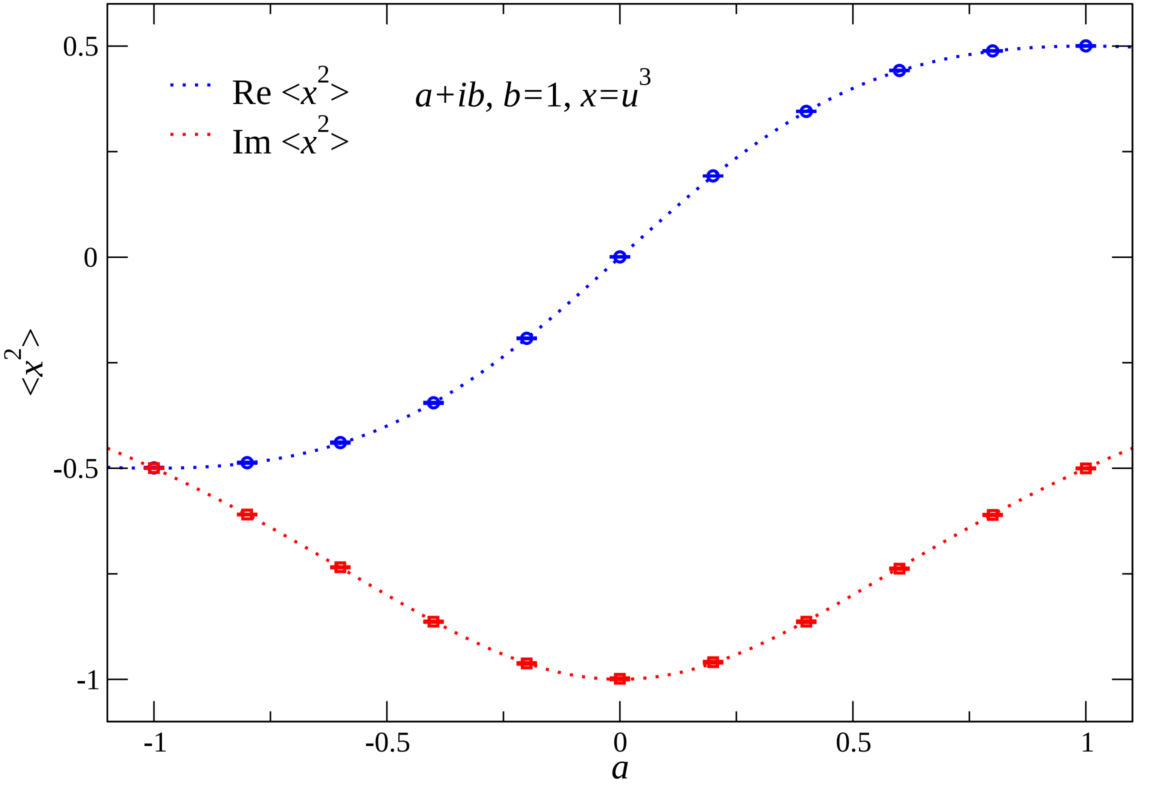


left: highly unstable

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

Field redefinitions: Gaussian

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



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

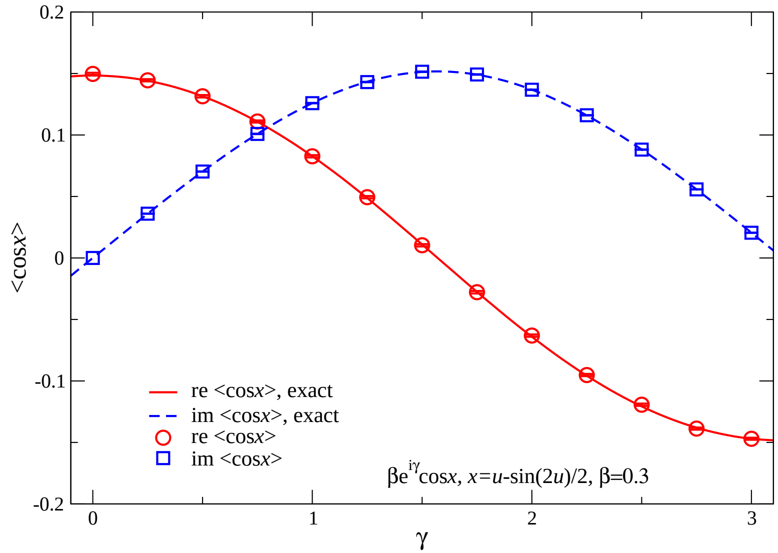
take also negative a

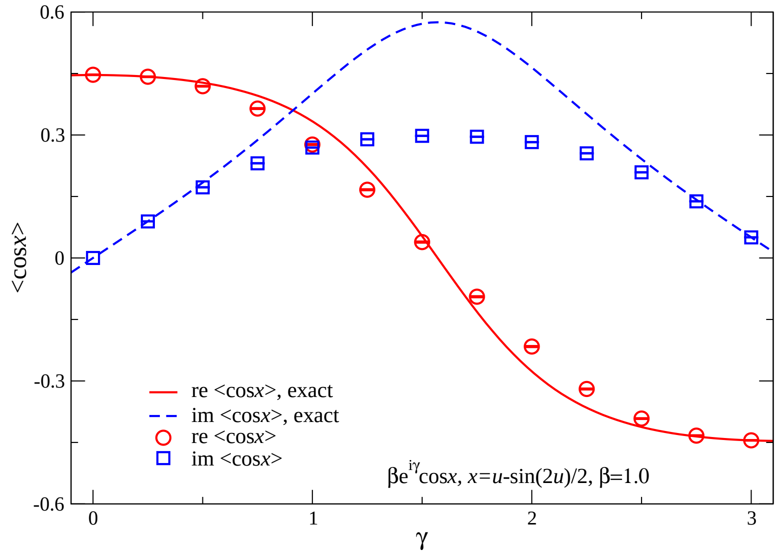
CLE finds the analytically continued answer to negative a!

Field redefinitions: from U(1) to SU(2)

$$Z_{\mathrm{U}(1)} = \int_{-\pi}^{\pi} dx\, e^{\beta \cos x} \qquad Z_{\mathrm{SU}(2)} = \int_{-\pi}^{\pi} dx\, \sin^2 x\, e^{\beta \cos x}$$

- transform U(1) model: $x(u) = u - \sin(2u)/2$
- generate SU(2) jacobian (!): $J(u) = x'(u) = 2\sin^2 u$





- stabilizes CLE at small complex $\beta = |\beta| e^{i\gamma}$
- some but very limited success in 3D XY model

Summary

complex Langevin can handle

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

however

- convergence: correct result not guaranteed

important

- stability of real manifold under complex fluctuations
- exploit freedom under field redefinitions and non-uniqueness of CLE

`see Denes' talk for SU(3) gauge theory`