FINITE DENSITY WITH COMPLEX LANGEVIN DYNAMICS

Gert Aarts

Swansea University

Swansea University
Prifysgol Abertawe

OUTLINE

- QCD phase diagram from the lattice ?
- sign problem at finite chemical potential

- a revived approach: stochastic quantization

- heavy dense QCD
- relativistic Bose gas and the Silver blaze problem
- instabilities and runaways

LATTICE QCD

IMPORTANCE SAMPLING

partition function: $$Z = \int DU\, D\bar{\psi} D\psi\, e^{-S} = \int DU\, e^{-S_B} \det M$$

- if $e^{-S_B} \det M > 0$, interpret as probability weight
- evaluate using importance sampling

LATTICE QCD

IMPORTANCE SAMPLING

partition function: $Z = \int DU\, D\bar{\psi} D\psi\, e^{-S} = \int DU\, e^{-S_B} \det M$

- if $e^{-S_B} \det M > 0$, interpret as probability weight
- evaluate using importance sampling

QCD at finite baryon chemical potential:

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

fermion determinant is complex!

- importance sampling not possible

sign problem

- basic tool of all lattice QCD algorithms breaks down

Why is the sign problem difficult?

PHASE QUENCHED THEORY

write $\det M = |\det M| e^{i\varphi}$

- phase quenched theory with weight $e^{-S_B} |\det M| > 0$
- observables:

$$\langle O \rangle_{\rm full} = \frac{\int DU\, e^{-S_B} \det M\, O}{\int DU\, e^{-S_B} \det M} = \frac{\langle e^{i\varphi} O \rangle_{\rm pq}}{\langle e^{i\varphi} \rangle_{\rm pq}}$$

WHY IS THE SIGN PROBLEM DIFFICULT?

PHASE QUENCHED THEORY

write $\det M = |\det M| e^{i\varphi}$ $\Omega =$ lattice volume

- phase quenched theory with weight $e^{-S_B} |\det M| > 0$
- observables:

$$\langle O \rangle_{\text{full}} = \frac{\int DU\, e^{-S_B} \det M\, O}{\int DU\, e^{-S_B} \det M} = \frac{\langle e^{i\varphi} O \rangle_{\text{pq}}}{\langle e^{i\varphi} \rangle_{\text{pq}}} \quad \rightarrow \quad \frac{0}{0} \quad \rightarrow \quad ??$$

- average phase factor

$$\langle e^{i\varphi} \rangle_{\text{pq}} = \frac{\int DU\, e^{-S_B} |\det M|\, e^{i\varphi}}{\int DU\, e^{-S_B} |\det M|} = \frac{Z_{\text{full}}}{Z_{\text{pq}}} = e^{-\Omega \Delta f} \rightarrow 0$$

overlap problem, exponentially hard in thermodynamic limit

QCD AT FINITE μ

SIGN 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
- how to pick the dominant configurations in the path integral?

QCD AT FINITE μ

SIGN 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
- how to pick the dominant configurations in the path integral?

radically different approach:

- complexifying all degrees of freedom: SU(3) $\rightarrow$ SL(3,$\mathbb{C}$)

stochastic quantization and complex Langevin dynamics

STOCHASTIC QUANTIZATION

LANGEVIN DYNAMICS

idea: Parisi & Wu '81

- path integral $Z = \int D\phi \, e^{-S}$
- do not interpret weight as a probability measure
- instead: equilibrium distribution of stochastic process

Brownian motion $\Leftrightarrow$ Langevin eq $\Leftrightarrow$ Fokker-Planck eq

- Langevin dynamics in "fifth" time direction

$$\frac{\partial \phi_x(\theta)}{\partial \theta} = -\frac{\delta S[\phi]}{\delta \phi_x(\theta)} + \eta_x(\theta)$$

- Gaussian noise $\langle \eta \rangle = 0 \quad \langle \eta_x(\theta) \eta_{x'}(\theta') \rangle = 2\delta_{xx'}\delta(\theta - \theta')$
- compute expectation values $\lim_{\theta \to \infty} \langle \phi_x(\theta) \phi_{x'}(\theta) \rangle$, etc

STOCHASTIC QUANTIZATION

LANGEVIN DYNAMICS

action and force $\delta S/\delta\phi$ complex: Parisi, Klauder '83

complexify Langevin dynamics

- example: real scalar field $\phi \rightarrow \phi^{\rm R} + i\phi^{\rm I}$
- Langevin eqs

$$\frac{\partial\phi^{\rm R}}{\partial\theta} = -{\rm Re}\,\frac{\delta S}{\delta\phi}\Big|_{\phi\rightarrow\phi^{\rm R}+i\phi^{\rm I}} + \eta$$

$$\frac{\partial\phi^{\rm I}}{\partial\theta} = -{\rm Im}\,\frac{\delta S}{\delta\phi}\Big|_{\phi\rightarrow\phi^{\rm R}+i\phi^{\rm I}}$$

- observables: analytic extension $\langle O(\phi)\rangle \rightarrow \langle O(\phi^{\rm R} + i\phi^{\rm I})\rangle$
- theoretical status not well-established (!)

READING MATERIAL

HISTORY

- original suggestion: Parisi & Wu ’81, Parisi, Klauder ’83
- overview: Damgaard and Hüffel, Physics Reports ’87
- finite μ for three-dimensional spin models:
  Karsch & Wyld PRL ’85, . . .
- renewed interest for Minkowski dynamics:
  Berges, Borsanyi, Sexty, Stamatescu ’05-’08

READING MATERIAL

THIS TALK

heavy dense QCD and related models:

- G.A. and I.O. Stamatescu: hep-lat/0807.1597, JHEP
  proceedings: hep-lat/0809.5527, hep-ph/0811.1850

Bose gas:

- G.A.: hep-lat/0810.2089, PRL, hep-lat/0902.4686, JHEP
  proceedings: hep-lat/0910.3772

instabilities:

- G.A., F. James, E. Seiler & I.O.S.: hep-lat/0912.0617, PLB

convergence:

- G.A., E.S. & I.O.S.: hep-lat/0912.3360
  G.A., F.J., E.S. & I.O.S.: in preparation

Heavy dense QCD

STATIC QUARKS

- bosonic action: standard SU(3) Wilson action

$$S_B = -\beta \sum_P \left(\frac{1}{6} \left[\mathrm{Tr}\, U_P + \mathrm{Tr}\, U_P^{-1} \right] - 1 \right)$$

- Wilson fermions in hopping expansion

$$\det M \approx \prod_{\mathbf{x}} \det \left(1 + h e^{\mu/T} \mathcal{P}_{\mathbf{x}} \right)^2 \det \left(1 + h e^{-\mu/T} \mathcal{P}_{\mathbf{x}}^{-1} \right)^2$$

with $h = (2\kappa)^{N_\tau}$ and (conjugate) Polyakov loops $\mathcal{P}_{\mathbf{x}}^{(-1)}$
static quarks propagate in temporal direction only

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

COMPLEX LANGEVIN DYNAMICS

Langevin update:

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

Gell-mann matrices λ_a ($a = 1, \ldots 8$)

- drift term

$$K_a = -D_a S_{\rm eff} \qquad S_{\rm eff} = S_B + S_F \qquad S_F = -\ln\det M$$

- noise

$$\langle\eta_a\rangle = 0 \qquad \langle\eta_a\eta_b\rangle = 2\delta_{ab}$$

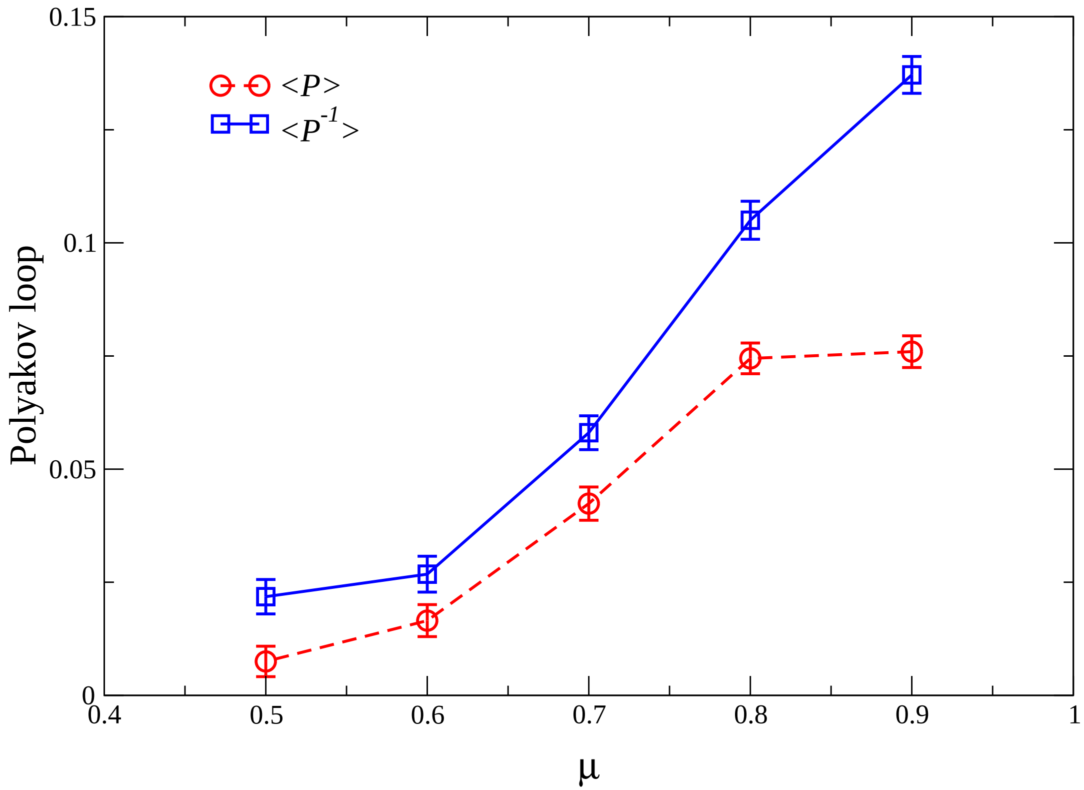
real action: $\Rightarrow K^\dagger = K \Leftrightarrow U \in$ SU(3)

complex action: $\Rightarrow K^\dagger \neq K \Leftrightarrow U \in$ SL(3,$\mathbb{C}$)

(conjugate) Polyakov loops

heavy dense QCD

first results on 4^4 lattice at $\beta = 5.6$, $\kappa = 0.12$, $N_f = 3$

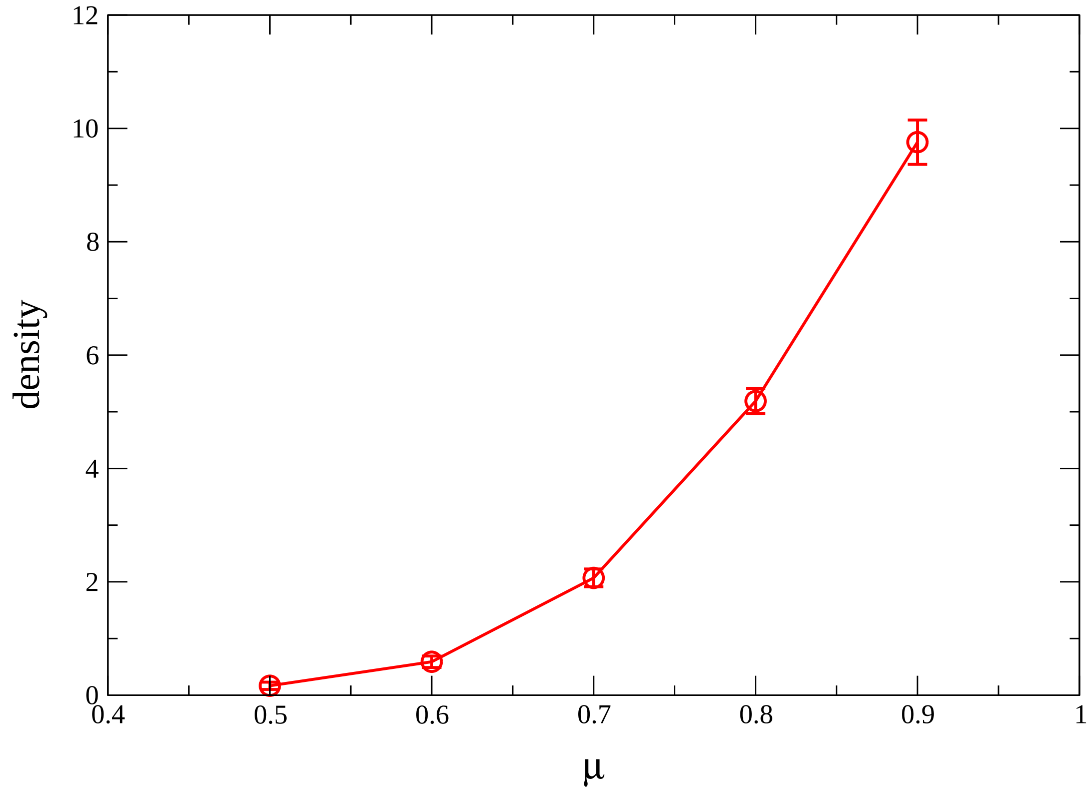


low-density "confining" phase $\Rightarrow$ high-density "deconfining" phase

DENSITY

HEAVY DENSE QCD

first results on 4^4 lattice at $\beta = 5.6$, $\kappa = 0.12$, $N_f = 3$



low-density phase $\Rightarrow$ high-density phase

SU(3) $\to$ SL(3,$\mathbb{C}$)

HEAVY DENSE QCD

- complex Langevin dynamics: no longer in SU(3)
- instead $U \in$ SL(3,$\mathbb{C}$)
- in terms of gauge potentials $U = e^{i\lambda_a A_a/2}$
  A_a is now complex
- how far from SU(3)?

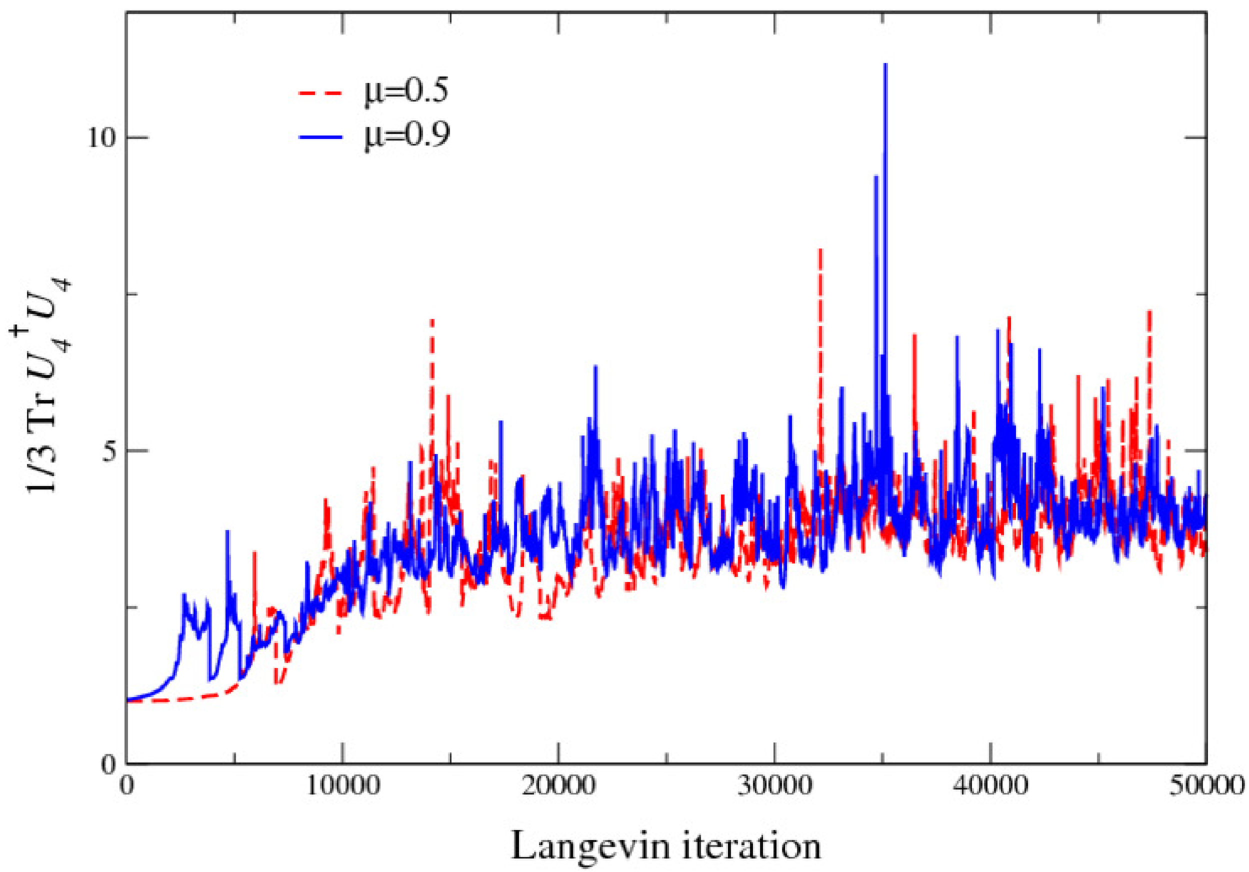
consider

$$\frac{1}{N}\mathrm{Tr}\, U^\dagger U \begin{cases} = 1 & \text{if } U \in \text{SU}(N) \\ \geq 1 & \text{if } U \in \text{SL}(N,\mathbb{C}) \end{cases}$$

SU(3) $\to$ SL(3,$\mathbb{C}$)

HEAVY DENSE QCD

$$\frac{1}{3}\mathrm{Tr}\, U^\dagger U \geq 1 \qquad\qquad = 1 \text{ if } U \in \text{SU(3)}$$



OVERLAP PROBLEM

HOW DOES IT WORK?

- most approaches start from $\mu = 0$ or $|\det M(\mu)|$
- complex Langevin dynamics radically different

visualization in simple U(1) model:

- $U = e^{ix}$ with $-\pi < x \leq \pi$
- complexification: $x \to x + iy$

$$S_B = -\frac{\beta}{2}\left(U + U^{-1}\right) = -\beta \cos x$$

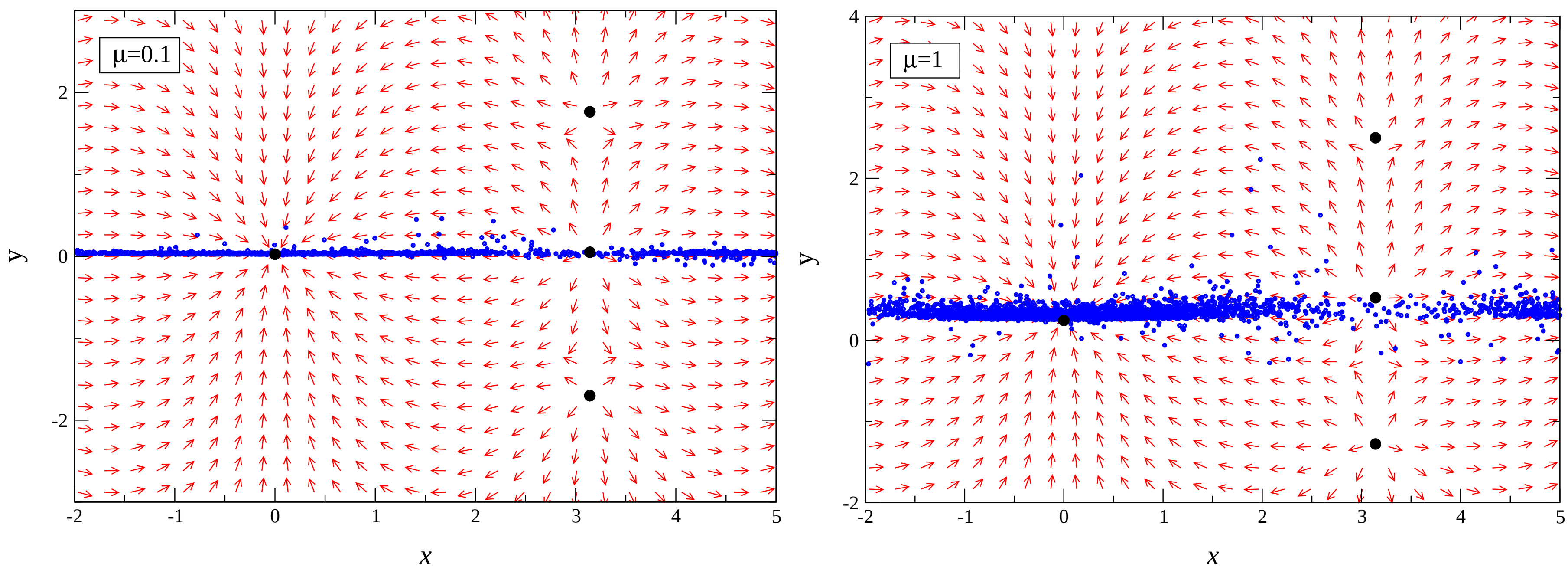
$$\det M = 1 + \frac{1}{2}\kappa\left[e^{\mu}U + e^{-\mu}U^{-1}\right] = 1 + \kappa\cos(x - i\mu)$$

partition function: $Z = \int_{-\pi}^{\pi} \frac{dx}{2\pi}\, e^{\beta\cos x}\left[1 + \kappa\cos(x - i\mu)\right]$

OVERLAP PROBLEM

HOW DOES IT WORK?

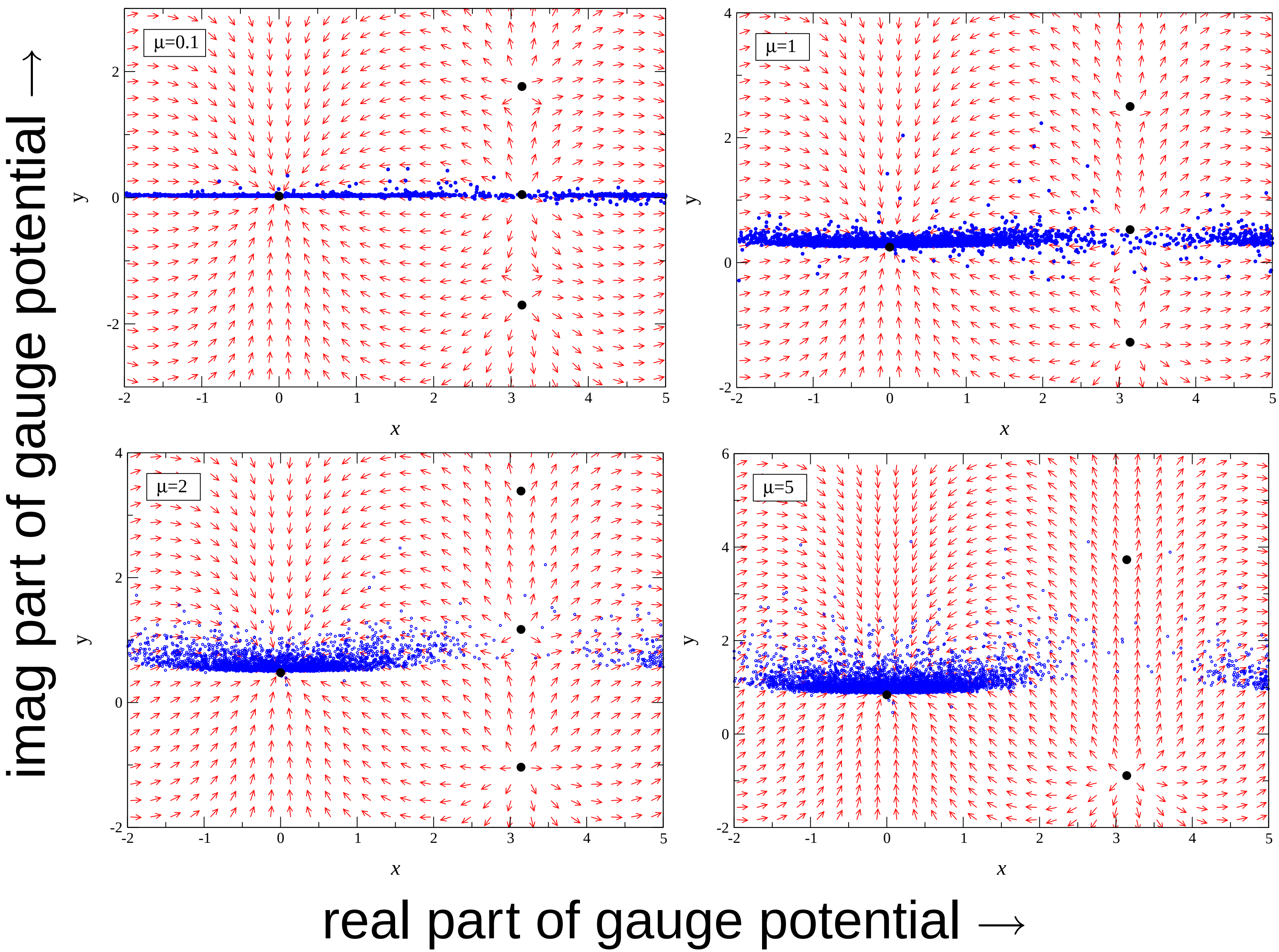
flow diagrams and Langevin evolution



- black dots: classical fixed points
- $\mu = 0$: dynamics only in x direction
- $\mu > 0$: spread in y direction

OVERLAP PROBLEM

HOW DOES IT WORK?



Phase transitions and the Silver Blaze

intriguing questions:

- how severe is the sign problem?
- thermodynamic limit?
- phase transitions?
- Silver Blaze problem? Cohen '03
- . . .

study in a model with a phase diagram with similar features as QCD at low temperature

$\Rightarrow$ relativistic Bose gas at nonzero μ

- scalar O(2) model with global symmetry
- lattice action

$$S = \sum_x \Big[\left(2d + m^2\right) \phi_x^* \phi_x + \lambda \left(\phi_x^* \phi_x\right)^2 - \sum_{\nu=1}^{4} \left(\phi_x^* e^{-\mu\delta_{\nu,4}} \phi_{x+\hat{\nu}} + \phi_{x+\hat{\nu}}^* e^{\mu\delta_{\nu,4}} \phi_x \right) \Big]$$

- complex scalar field, $d = 4$, $m^2 > 0$
- $S^*(\mu) = S(-\mu^*)$ as in QCD

also studied by Endres using worldline formulation hep-lat/0610029

Relativistic Bose gas

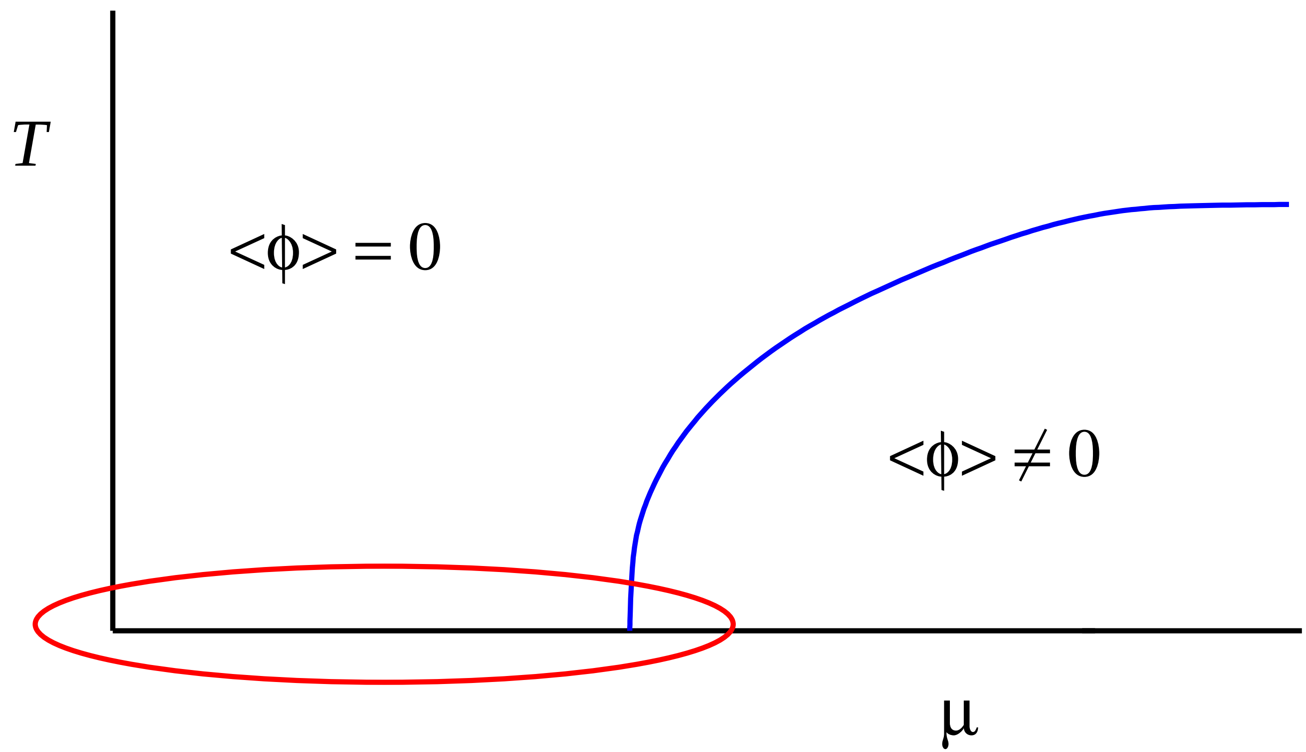
phase transitions and the Silver Blaze

nonderivative terms at tree level in the continuum

$$V(\phi) = (m^2 - \mu^2)|\phi|^2 + \lambda|\phi|^4$$

condensation when $\mu^2 > m^2$, SSB

Silver Blaze problem



RELATIVISTIC BOSE GAS

COMPLEX LANGEVIN

- write $\phi = (\phi_1 + i\phi_2)/\sqrt{2} \quad \Rightarrow \quad \phi_a \quad (a = 1, 2)$
- complexification $\phi_a \quad \rightarrow \quad \phi_a^{\rm R} + i\phi_a^{\rm I}$
- complex Langevin equations

$$\frac{\partial \phi_a^{\rm R}}{\partial \theta} = -{\rm Re}\,\frac{\delta S}{\delta \phi_a}\Big|_{\phi_a \to \phi_a^{\rm R} + i\phi_a^{\rm I}} + \eta_a$$

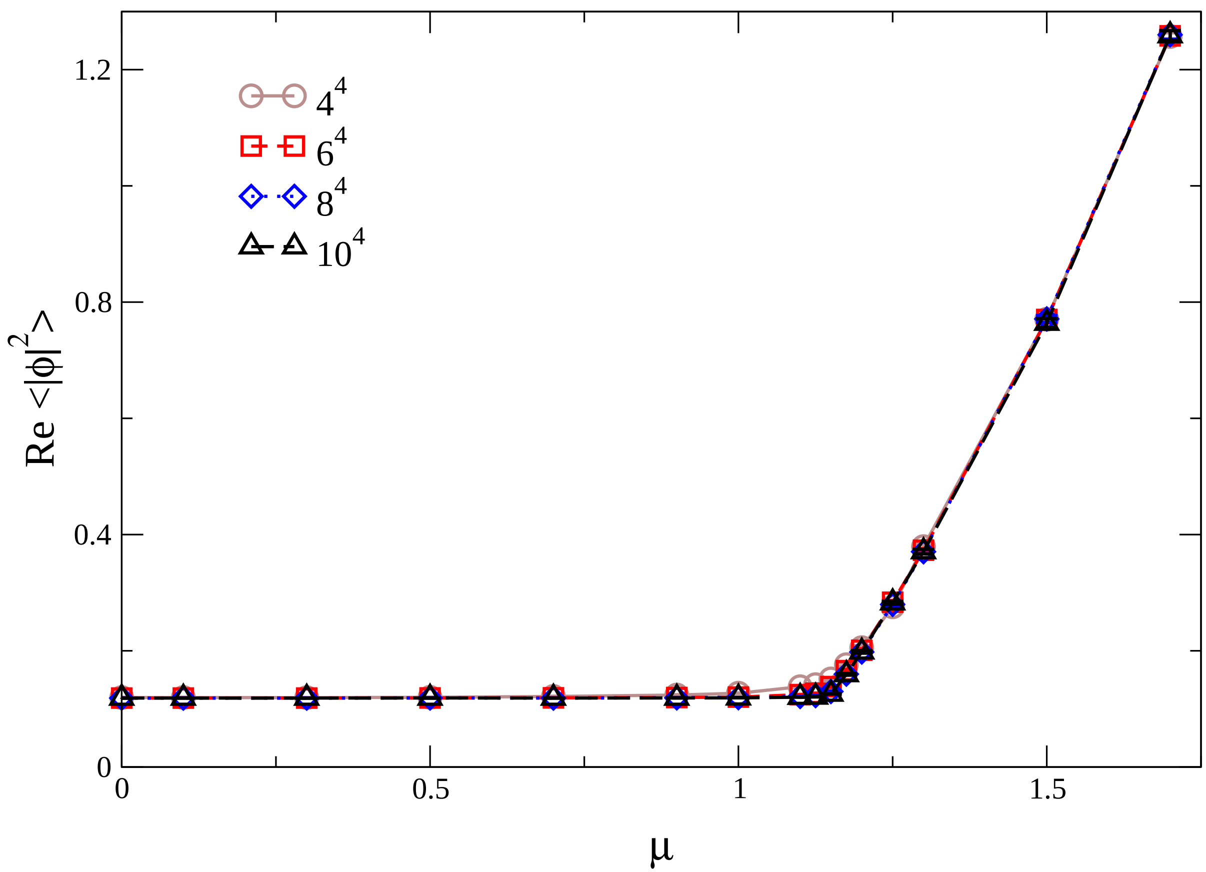
$$\frac{\partial \phi_a^{\rm I}}{\partial \theta} = -{\rm Im}\,\frac{\delta S}{\delta \phi_a}\Big|_{\phi_a \to \phi_a^{\rm R} + i\phi^{\rm I}}$$

- straightforward to solve numerically, $m = \lambda = 1$
- lattices of size N^4, with $N = 4, 6, 8, 10$

RELATIVISTIC BOSE GAS

COMPLEX LANGEVIN

field modulus squared $$|\phi|^2 \to \frac{1}{2}\left({\phi_a^{\rm R}}^2 - {\phi_a^{\rm I}}^2\right) + i\phi_a^{\rm R}\phi_a^{\rm I}$$

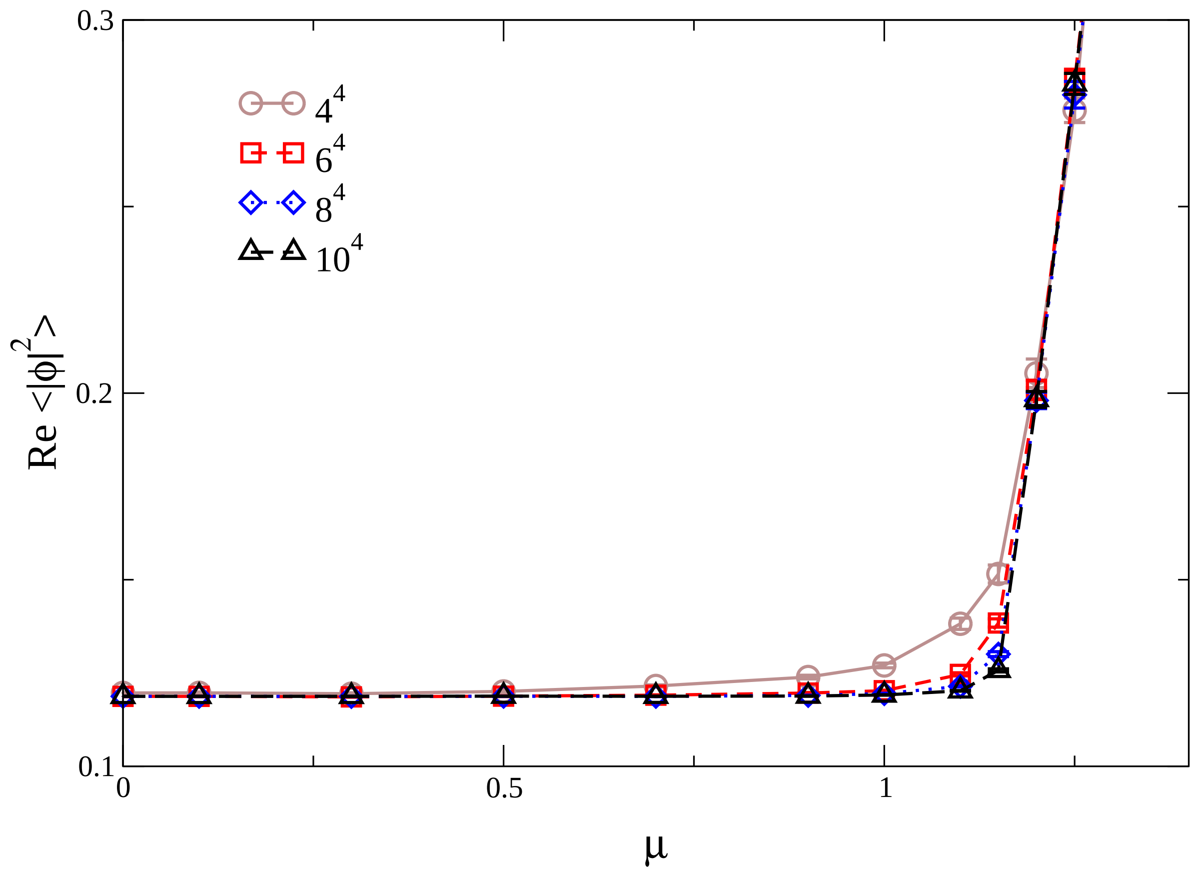


Silver Blaze!

RELATIVISTIC BOSE GAS

COMPLEX LANGEVIN

field modulus squared $$|\phi|^2 \to \frac{1}{2}\left({\phi_a^{\rm R}}^2 - {\phi_a^{\rm I}}^2\right) + i\phi_a^{\rm R}\phi_a^{\rm I}$$

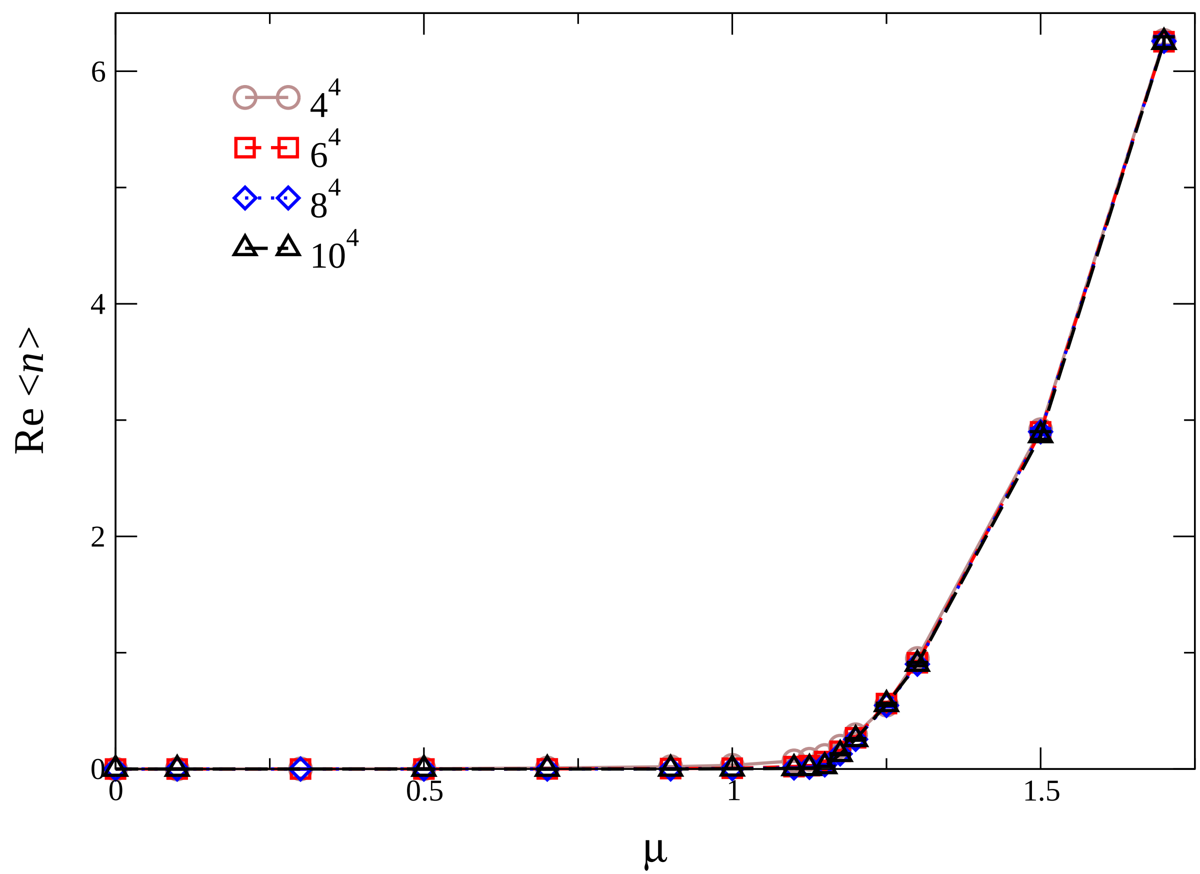


second order phase transition in thermodynamic limit

RELATIVISTIC BOSE GAS

COMPLEX LANGEVIN

density $\langle n \rangle = (1/\Omega)\partial \ln Z/\partial\mu$

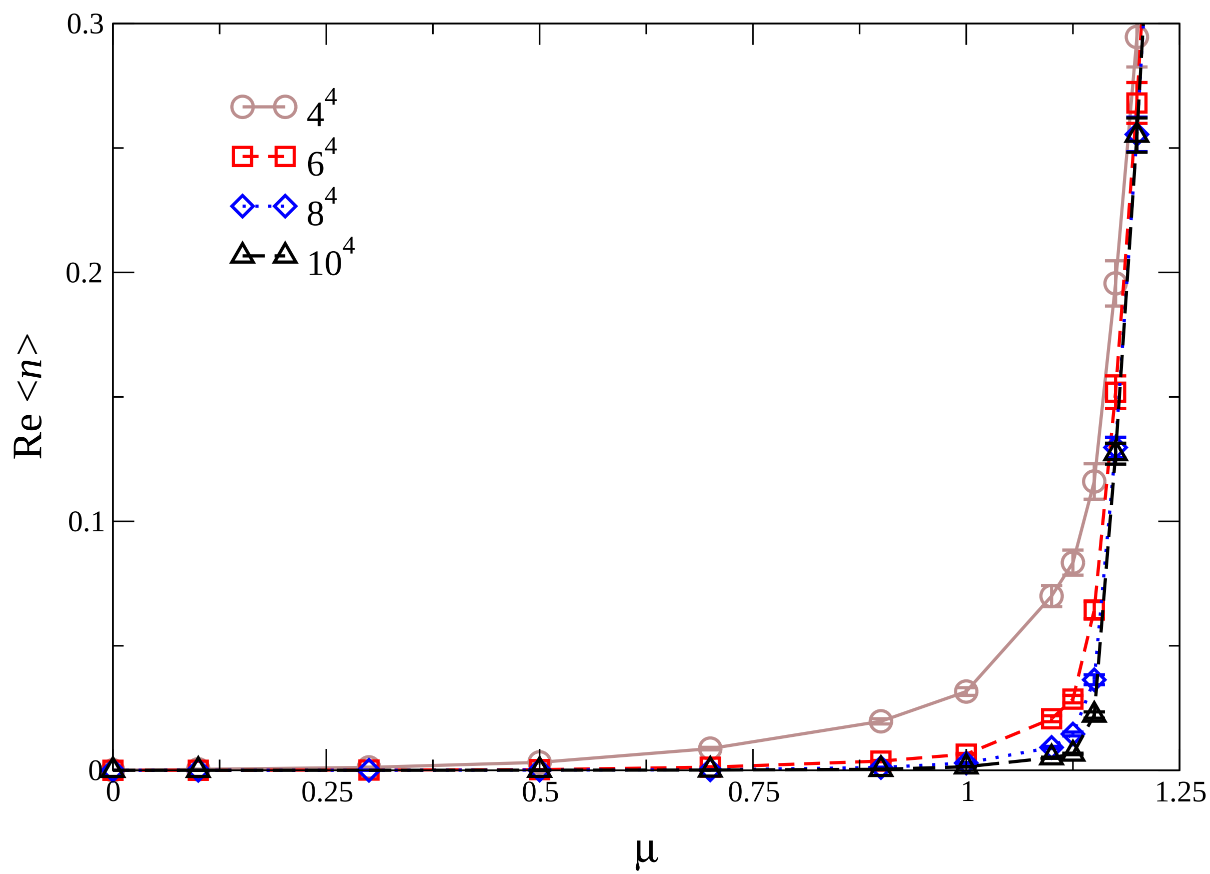


Silver Blaze

RELATIVISTIC BOSE GAS

COMPLEX LANGEVIN

density $\langle n \rangle = (1/\Omega)\partial \ln Z/\partial\mu$



second order phase transition in thermodynamic limit

SILVER BLAZE AND THE SIGN PROBLEM

RELATIVISTIC BOSE GAS

Silver Blaze and sign problems are intimately related

- complex action: $e^{-S} = |e^{-S}|e^{i\varphi}$
- phase quenched theory $Z_{\rm pq} = \int D\phi |e^{-S}|$

physics of phase quenched theory:

- chemical potential appears only in mass parameter (in continuum notation)

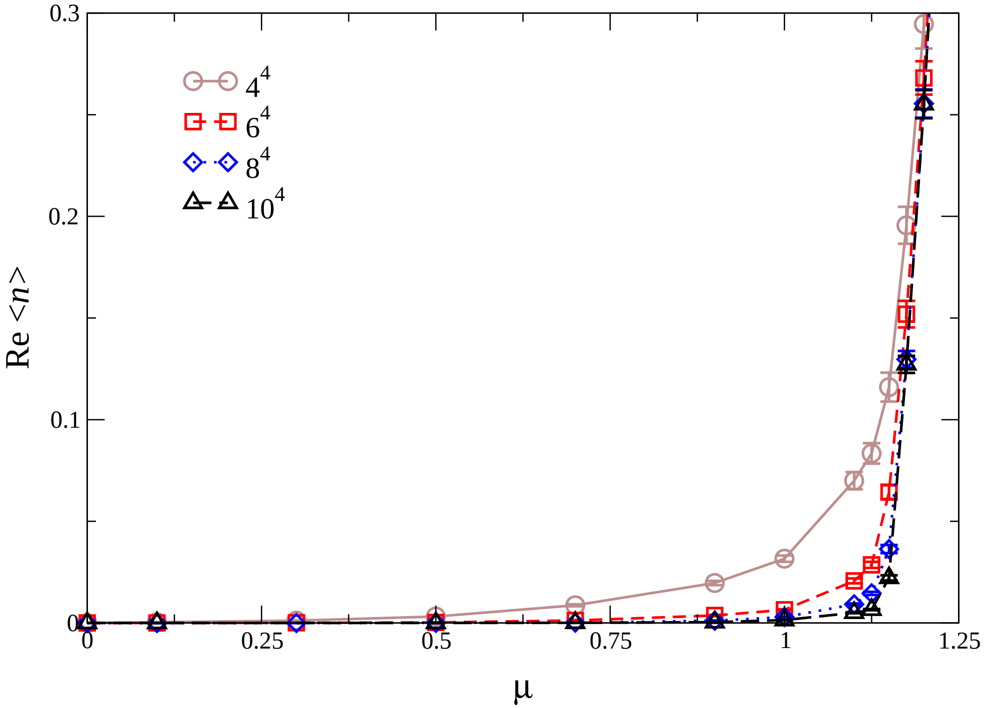
$$V = (m^2 - \mu^2)|\phi|^2 + \lambda|\phi|^4$$

- dynamics of symmetry breaking, no Silver Blaze

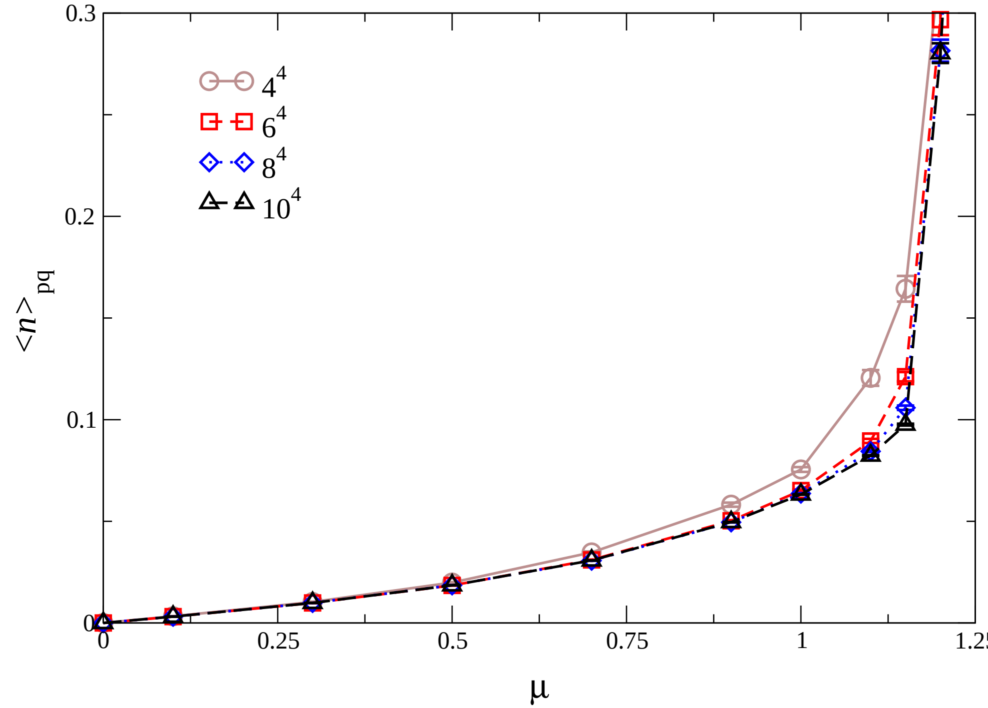
Silver Blaze and the sign problem

complex vs phase quenched

density



complex



phase quenched

phase $e^{i\varphi} = e^{-S}/|e^{-S}|$ does precisely what is expected

HOW SEVERE IS THE SIGN PROBLEM?

AVERAGE PHASE FACTOR

- complex action $e^{-S} = |e^{-S}|e^{i\varphi}$

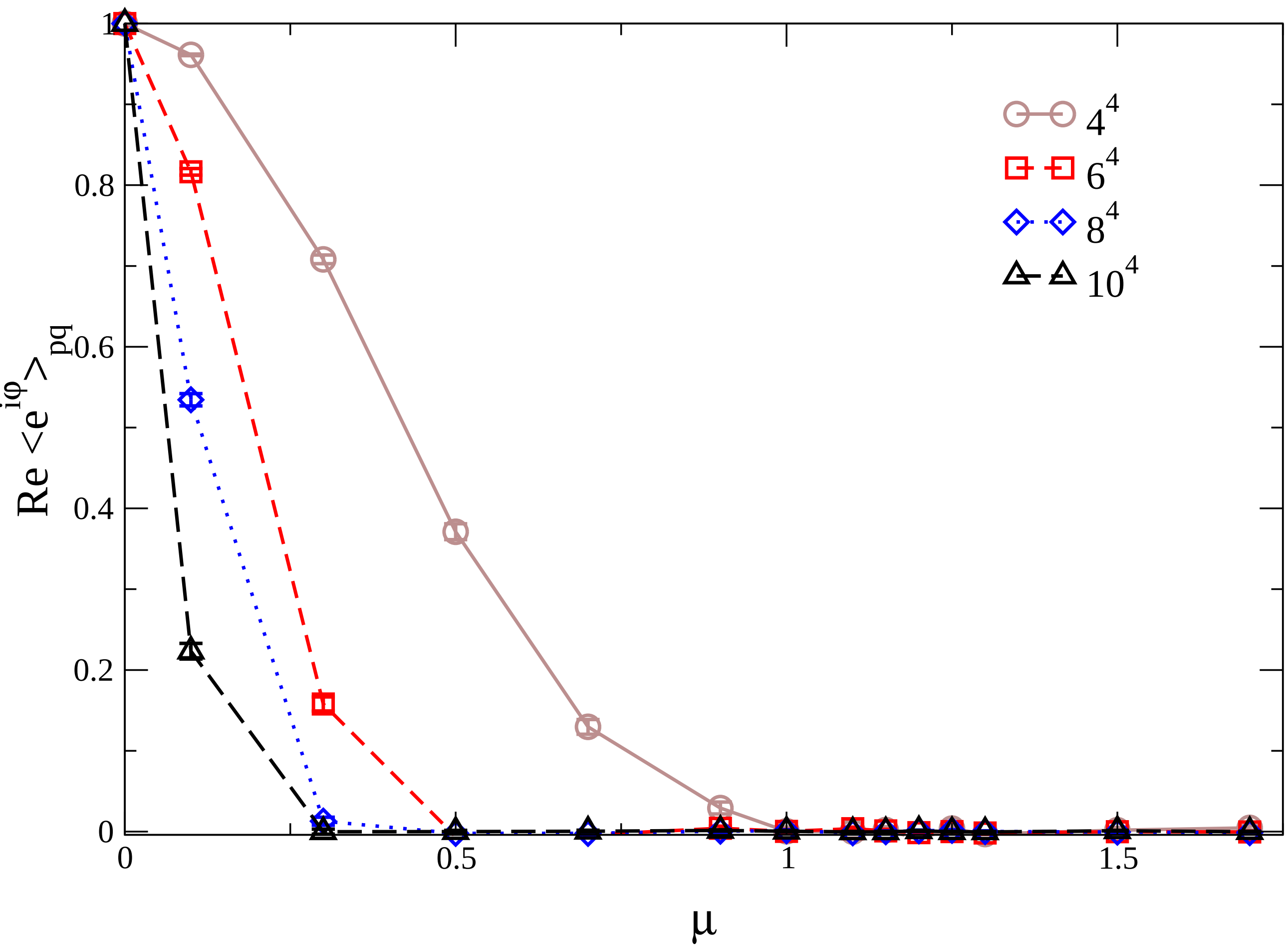
- average phase factor in phase quenched theory

$$\langle e^{i\varphi} \rangle_{\rm pq} = \frac{Z_{\rm full}}{Z_{\rm pq}} = e^{-\Omega \Delta f} \to 0 \quad \text{as} \quad \Omega \to \infty$$

- exponentially hard in thermodynamic limit

How severe is the sign problem?

AVERAGE PHASE FACTOR



average phase factor $\langle e^{i\varphi} \rangle_{\rm pq}$

INSTABILITIES

old problem from the 80s: instabilities and runaways

- unstable classical trajectories
- force not always restoring
- noise should kick trajectories of unstable paths.

careful integration mandatory

adaptive stepsize

- XY model at nonzero μ and heavy dense QCD

INSTABILITIES

XY MODEL

three-dimensional XY model at nonzero μ

$$S = -\beta \sum_x \sum_{\nu=0}^{2} \cos\left(\phi_x - \phi_{x+\hat{\nu}} - i\mu\delta_{\nu,0}\right)$$

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

unexpectedly difficult to simulate with complex Langevin!

numerics shares many features with heavy dense QCD

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

INSTABILITIES

XY MODEL

- classical forces

$$K_x^{\mathrm{R}} = -\mathrm{Re}\frac{\partial S}{\partial \phi_x}$$
$$K_x^{\mathrm{I}} = -\mathrm{Im}\frac{\partial S}{\partial \phi_x}$$

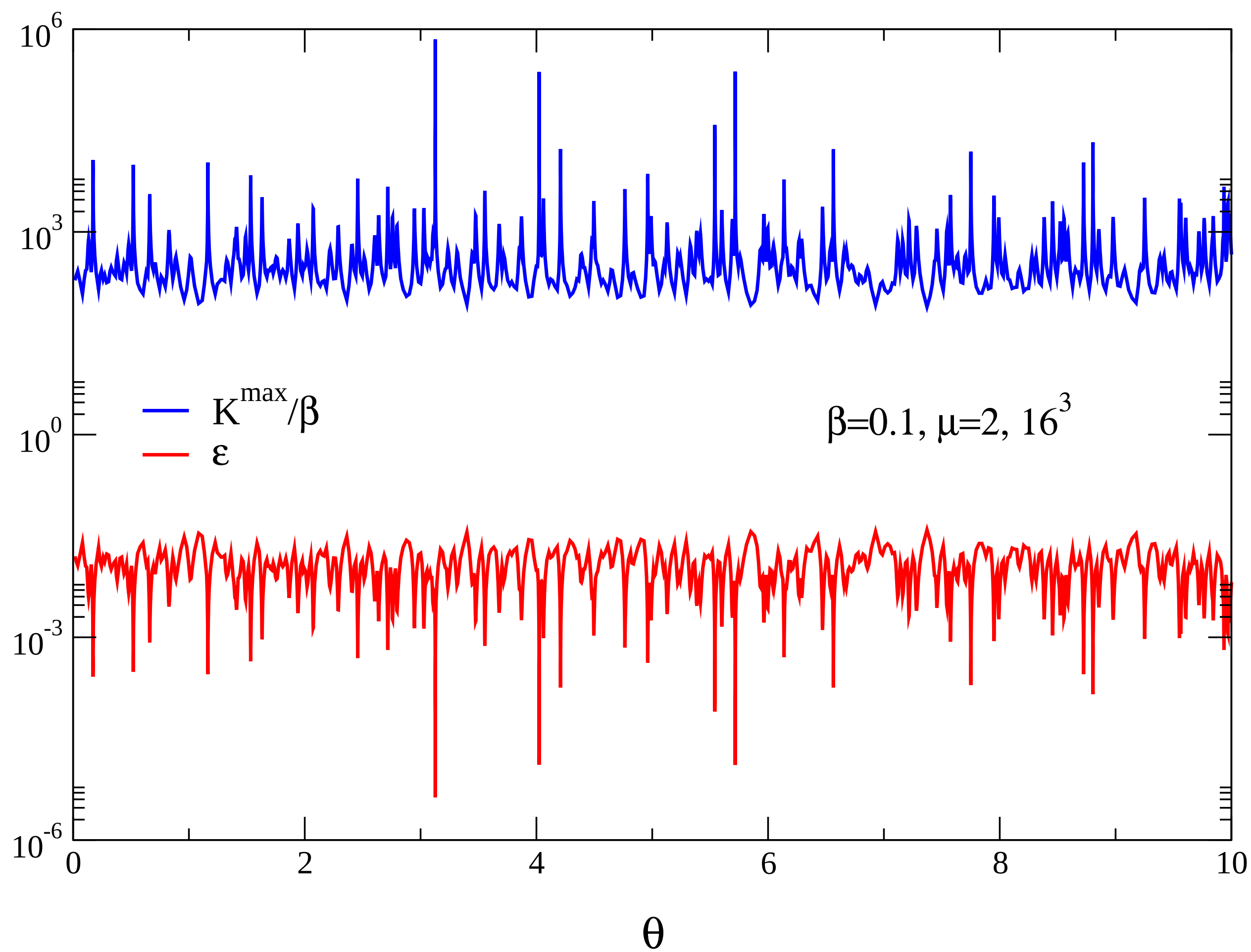
- restrict maximal step $\epsilon \, K^{\mathrm{max}}$

large force $\Leftrightarrow$ small stepsize

INSTABILITIES

XY MODEL

$K^{\max}$ and adaptive time step during the evolution



INSTABILITIES

XY MODEL

$K^{\max}$ behaves as expected:

- fluctuates over several orders of magnitude
- fluctuations increase with volume:
  more potentially unstable trajectories
- stepsize has to be small occasionally but recovers

with adaptive stepsize: no instabilities encountered!

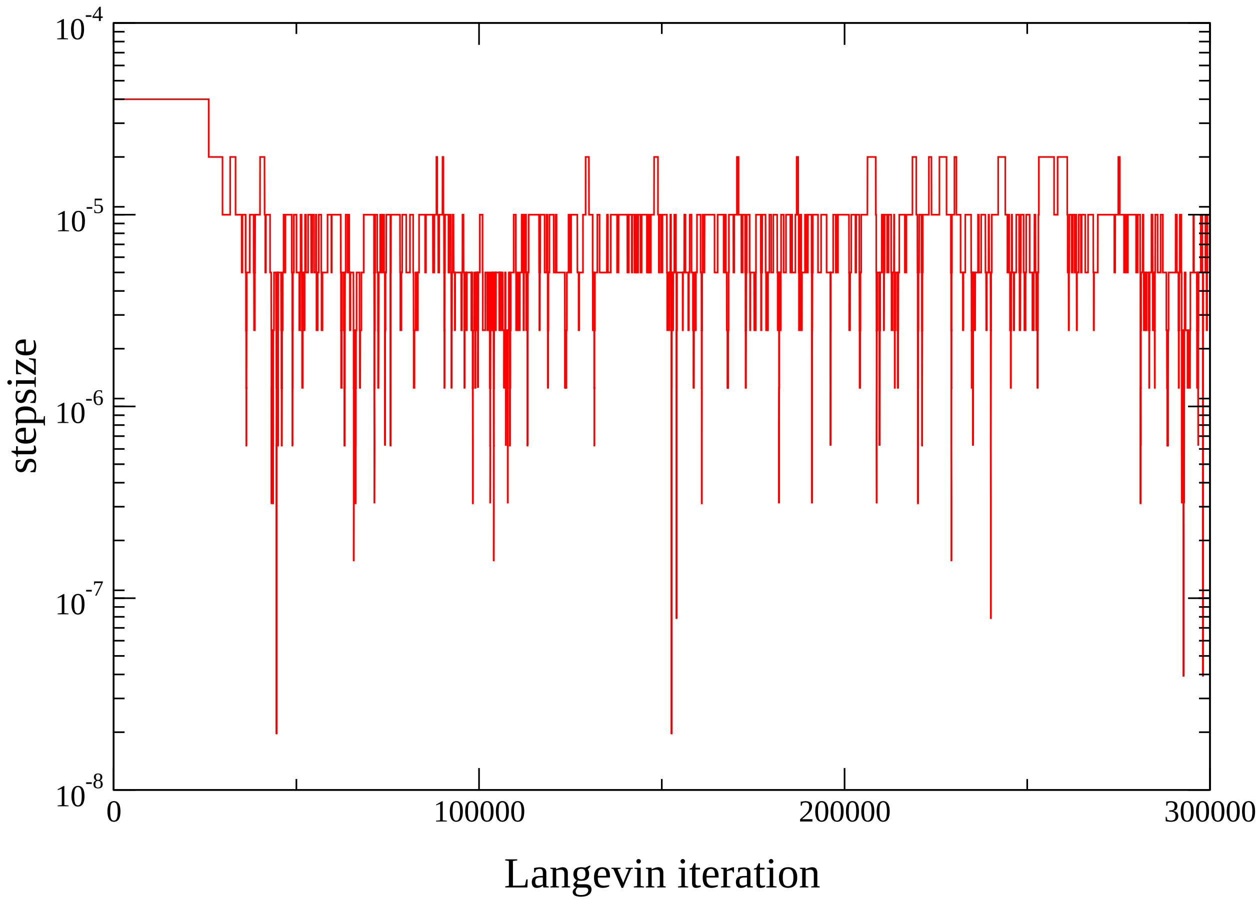
many very long runs for wide range of parameters

with fixed stepsize: impossible to generate a thermalized configuration!

INSTABILITIES

HEAVY DENSE QCD, $\beta = 5, \kappa = 0.12, \mu = 0.7, 2^4$

same is true for heavy dense QCD

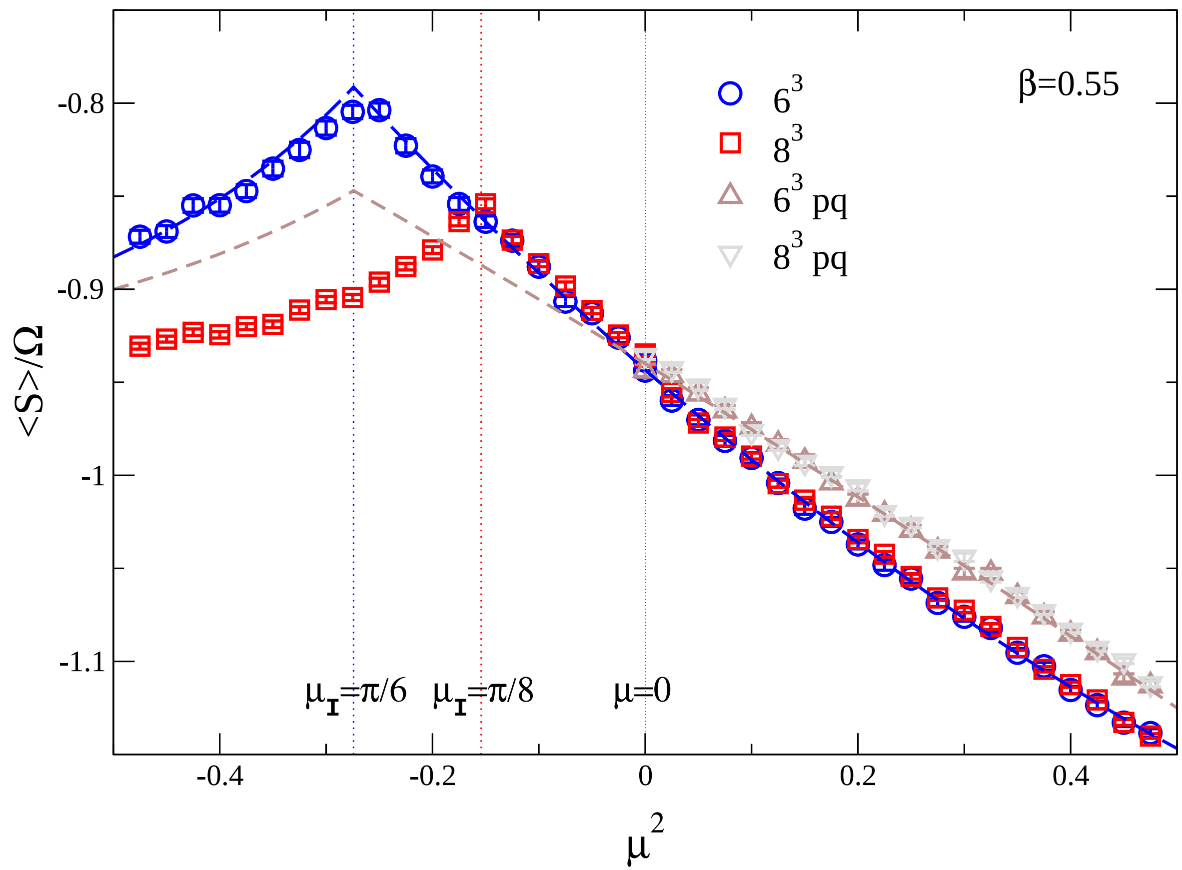


occasionally *very* small stepsize required
can go to longer Langevin times without problems

XY MODEL

PHYSICS RESULT

action density in the magnetized phase ($\beta = 0.55$)



real μ ($\mu^2 > 0$) imaginary μ ($\mu^2 < 0$) and phase quenched

XY MODEL

PHYSICS RESULT

- real and imag μ results analytic in μ^2
- phase quenched result distinctly different

imaginary μ:

- “Roberge-Weiss” transition at $\mu_{\rm I} = \pi/N_\tau$ (center symmetry is trivial)

SUMMARY

FINITE CHEMICAL POTENTIAL

many stimulating results:

complex Langevin can handle

- sign problem
- Silver Blaze problem
- nonabelian dynamics
- phase transition
- thermodynamic limit
- SU(3) $\rightarrow$ SL(3,$\mathbb{C}$)

problems from the 80s:

- instabilities and runaways $\rightarrow$ adaptive stepsize
- convergence to correct result: *can* be highly nontrivial

  hep-lat/0912.3360