A study of the XY model at finite chemical potential using complex Langevin dynamics

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Motivation

- Adding chemical potential makes action complex

$$S^*(\mu) = S(-\mu^*)$$

- QCD: Fermion determinant complex

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

- Difficult to treat nonperturbatively
- Can't interpret weight $e^{-S} = \left|e^{-S}\right| e^{i\varphi}$ as a probability

Sign problem

How to deal with complex phase $e^{i\varphi}$?

- Ignore it (*phase quenched approximation*)

$$Z_{\text{pq}} = \int D\phi \left| e^{-S} \right|$$

  - Problem: not sampling from correct distribution
  - Different physics
- Apply reweighting
  - Problem: Reweighting fails if $\langle e^{i\varphi} \rangle_{\text{pq}} \sim 0$
  - But phase vanishes exponentially in thermodynamic limit (Ω volume)

$$\langle e^{i\varphi} \rangle_{\text{pq}} = \frac{Z}{Z_{\text{pq}}} \sim e^{-\Omega \Delta f}$$

- Need alternative approach

Langevin dynamics

Parisi & Wu, '81

- Classical field equation $\frac{\delta S[\phi]}{\delta \phi} = 0$
- Add fictitious time dimension ϑ, $\phi \longrightarrow \phi(\vartheta)$
- Random kicks add fluctuations
- Equation of motion *Langevin equation*

$$\frac{\partial \phi}{\partial \vartheta} = -\frac{\delta S}{\delta \phi} + \eta(\vartheta)$$

- Uncorrelated noise $\langle \eta(\vartheta) \rangle = 0, \quad \langle \eta(\vartheta)\eta(\vartheta') \rangle = 2\delta(\vartheta - \vartheta')$

Langevin dynamics

- Formal proof of stable distribution
- Equilibrium probability distribution $\rho[\phi] \sim e^{-S[\phi]}$
- Noise averages equal to expectation values in limit $\vartheta \to \infty$

$$\lim_{\vartheta \to \infty} \langle O(\phi) \rangle_\eta = \frac{1}{Z} \int D\phi O(\phi) e^{-S[\phi]}$$

- *No importance sampling*

Complex Langevin dynamics

- What if $S[\phi]$ complex?
- Drift term becomes complex

$$\frac{\delta S}{\delta \phi} = \mathrm{Re}\frac{\delta S}{\delta \phi} + i\mathrm{Im}\frac{\delta S}{\delta \phi}$$

- All field variables *complexify* into expanded complex space

$$\phi \rightarrow \phi^{\mathrm{R}} + i\phi^{\mathrm{I}}$$

- Also for observables $\langle O(\phi)\rangle \rightarrow \langle O(\phi^{\mathrm{R}} + i\phi^{\mathrm{I}})\rangle$
- Distribution extends into complexified space, no formal proof of convergence

$$\rho[\phi] \rightarrow P[\phi^{\mathrm{R}}, \phi^{\mathrm{I}}]$$

Parisi, Klauder '83

Complexified numerical updates

- Discretize Langevin time $\vartheta = n\epsilon$
- Force terms

$$K^{\mathrm{R}} = -\mathrm{Re}\left.\frac{\delta S}{\delta\phi}\right|_{\phi\to\phi^{\mathrm{R}}+i\phi^{\mathrm{I}}} \quad K^{\mathrm{I}} = -\mathrm{Im}\left.\frac{\delta S}{\delta\phi}\right|_{\phi\to\phi^{\mathrm{R}}+i\phi^{\mathrm{I}}}$$

- Langevin equation of motion

$$\begin{aligned}\phi^{\mathrm{R}}(n+1) =& \phi^{\mathrm{R}}(n) + \epsilon K^{\mathrm{R}}(n) + \sqrt{\epsilon}\eta(n)\\ \phi^{\mathrm{I}}(n+1) =& \phi^{\mathrm{I}}(n) + \epsilon K^{\mathrm{I}}(n)\end{aligned}$$

- Real noise $\langle\eta(n)\rangle = 0 \quad \langle\eta(n)\eta(n')\rangle = 2\delta_{n,n'}$

Problems since eighties

- No formal proof of convergence to correct distribution e^{-S}
- Runaway solutions and instabilities — Ambjorn et al '86
  - Solved using an adaptive stepsize
- Convervence to incorrect result — Ambjorn et al '86
  - This work
  - Also recent studies with complex noise
- Also expected to be present in QCD
- XY model:
  - Both features present
  - Easier to simulate than QCD
  - Reformulation without sign problem (world line method) Banerjee & Chandrasekharan, 2010

XY model

- Each site x associtate an angle $\phi \in [0, 2\pi)$

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

- Chemical potential couples to symmetry $\phi \to \phi + \alpha$
- Well understood at $\mu = 0$:
  - Phase transition at $\beta_c = 0.454$
  - $\beta > \beta_c$ ordered phase (spins aligned)
  - $\beta < \beta_c$ disordered phase

XY model

- Complexified force terms unbounded

$$K_x^{\mathrm{R}} = -\beta \sum_{\nu} \sin(\phi_x^{\mathrm{R}} - \phi_{x+\hat{\nu}}^{\mathrm{R}}) \cosh(\phi_x^{\mathrm{I}} - \phi_{x+\hat{\nu}}^{\mathrm{I}} - \mu\delta_{\nu,0}) +$$
$$\sin(\phi_x^{\mathrm{R}} - \phi_{x-\hat{\nu}}^{\mathrm{R}}) \cosh(\phi_x^{\mathrm{I}} - \phi_{x-\hat{\nu}}^{\mathrm{I}} + \mu\delta_{\nu,0})$$
$$K_x^{\mathrm{I}} = -\beta \sum_{\nu} \cos(\phi_x^{\mathrm{R}} - \phi_{x+\hat{\nu}}^{\mathrm{R}}) \sinh(\phi_x^{\mathrm{I}} - \phi_{x+\hat{\nu}}^{\mathrm{I}} - \mu\delta_{\nu,0}) +$$
$$\cos(\phi_x^{\mathrm{R}} - \phi_{x-\hat{\nu}}^{\mathrm{R}}) \sinh(\phi_x^{\mathrm{I}} - \phi_{x-\hat{\nu}}^{\mathrm{I}} + \mu\delta_{\nu,0})$$

- When $\mu = 0$, $\phi^{\mathrm{I}} = 0$

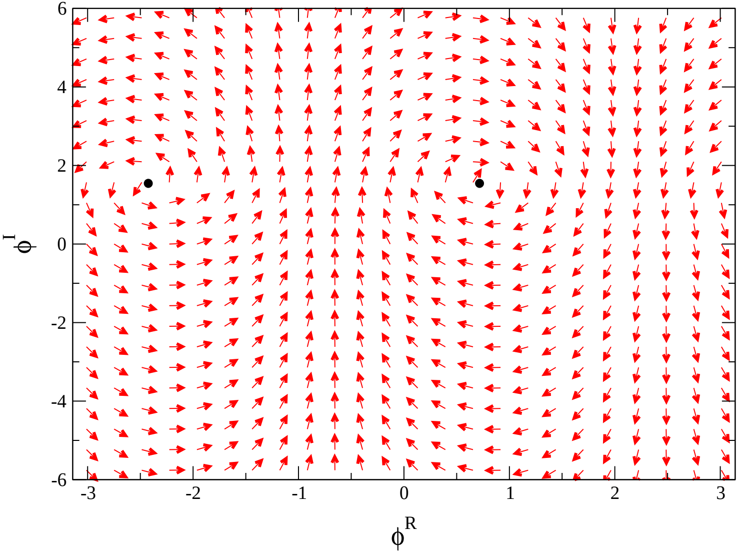
$$\left|K^{\mathrm{R}}\right| \leq 6\beta \quad K^{\mathrm{I}} = 0$$

Instabilities and runaways

Aarts, FJ, Seiler, Stamatescu, PLB hep-lat/09120617

- Long known that sometimes ϕ^{I} goes to infinity
- Extra imaginary dimension ϕ^{I} unbounded
  - $\Rightarrow$ Forces can "blow up"
- Classical flow diagram of $(K^{\mathrm{R}}, K^{\mathrm{I}})$ shows fixed points and unstable directions
- Random kicks can send ϕ^{I} along these to infinity

Classical flow example



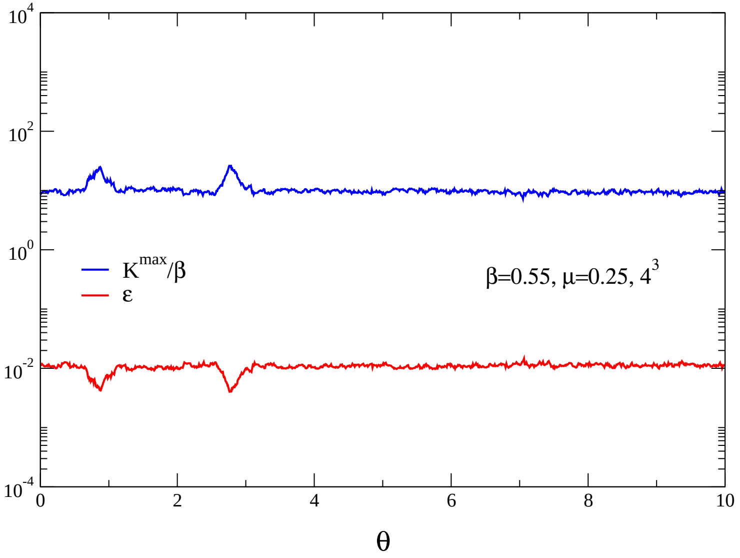
Adaptive stepsize

- Recently observed that reduction in ϵ almost eliminates runaways Berges &Stamatescu 2005
- Problem appears when product ϵK large
- Solution: reduce ϵ when large force $K^{\max} = \max_x \left| K_x^{\mathrm{R}} + iK_x^{\mathrm{I}} \right|$
- Take

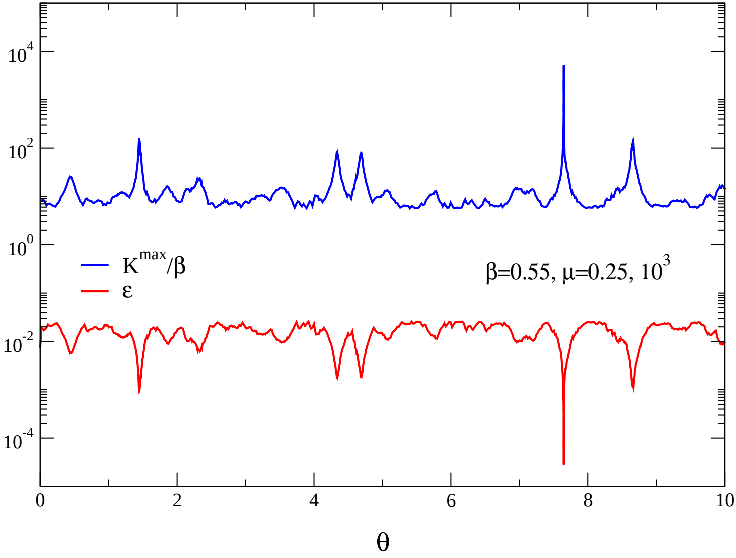
$$\epsilon_n = \bar{\epsilon} \frac{\langle K^{\max} \rangle}{K_n^{\max}}$$

- With $\bar{\epsilon}$ given, $\langle K^{\max} \rangle$ precomputed/computed during thermalisation
- Similar algorithm implemented with heavy dense QCD
- All cases tested, completely eliminates runaway solutions

$\Omega = 4^3$

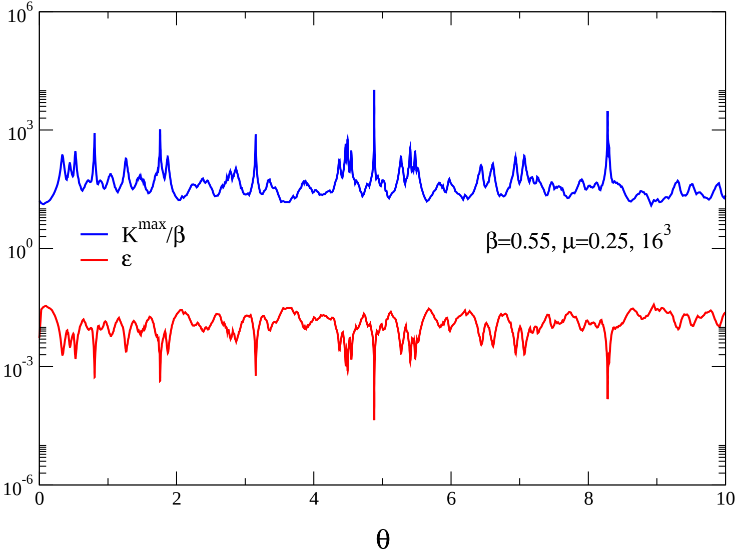


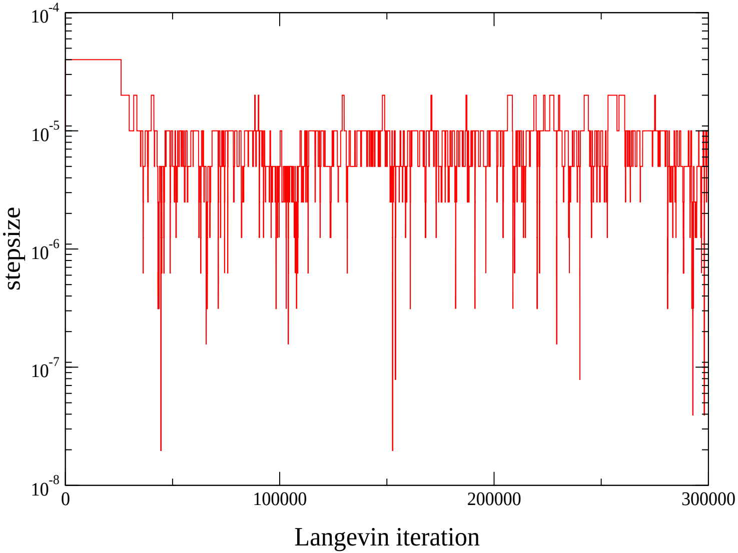
$\Omega = 10^3$



10^4
10^2
10^0
10^{-2}
10^{-4}
K^{max}/β
ε
β=0.55, μ=0.25, 10^3
0
2
4
6
8
10
θ

$\Omega = 16^3$




stepsize
Langevin iteration
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
0
100000
200000
300000

Convergence

- Known since '80s that complex Langevin can converge to "wrong" value Ambjorn et al '86
- Recent studies using complex noise found correct convergence only when noise purely real Aarts et al hep-lat/0912.3360
- Strategy: compare $\langle S \rangle$ with known results Aarts & FJ hep-lat/1005.3468
  - Small μ: take imaginary chemical potential, continue over $\mu^2 \sim 0$
  - Comparison with alternative result: world line method Banerjee & Chandrasekharan

Imaginary chemical potential

- Choose $\mu = i\mu_I$
- Action becomes

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

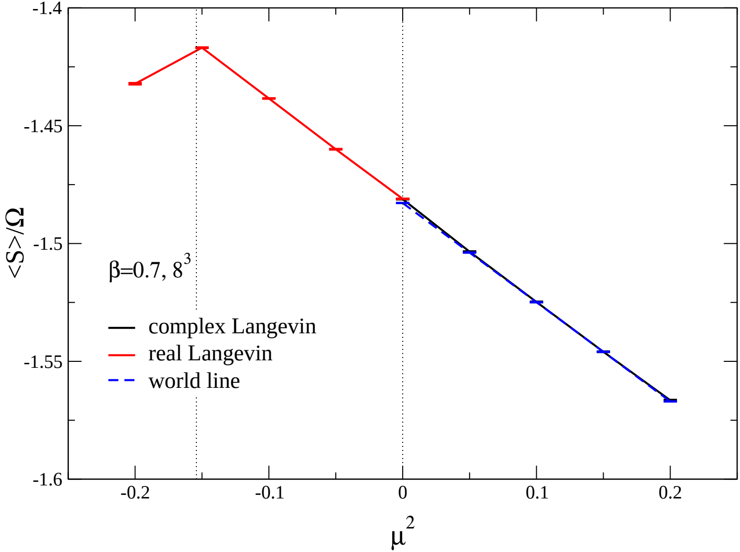
- Action now *real*
- Standard techniques can apply
- Can shift μ_I to boundry conditions
- Roberge-Weiss transition at $\mu_I = \pi/N_\tau$

Comparison with world line

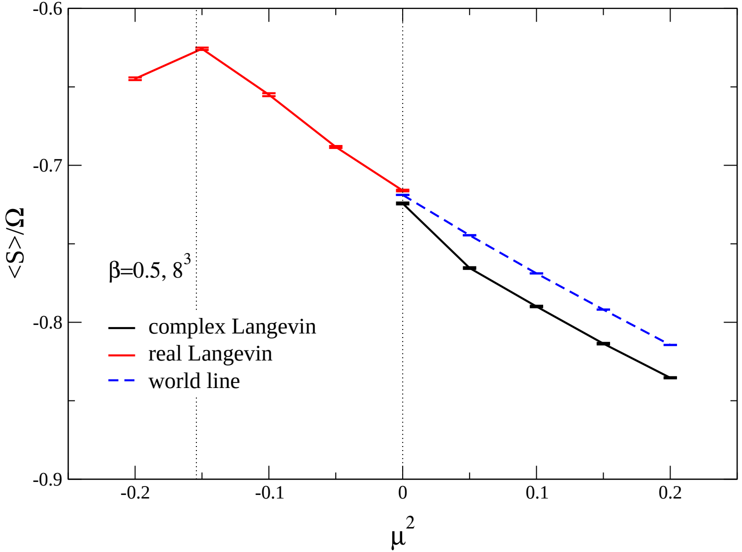
Banerjee, Chandrasekhran hep-lat/1001.3648

- Rewrite original action
- Make a duality transform of field variables
- Circumvents sign problem
- Efficiently solved with worm algorithm

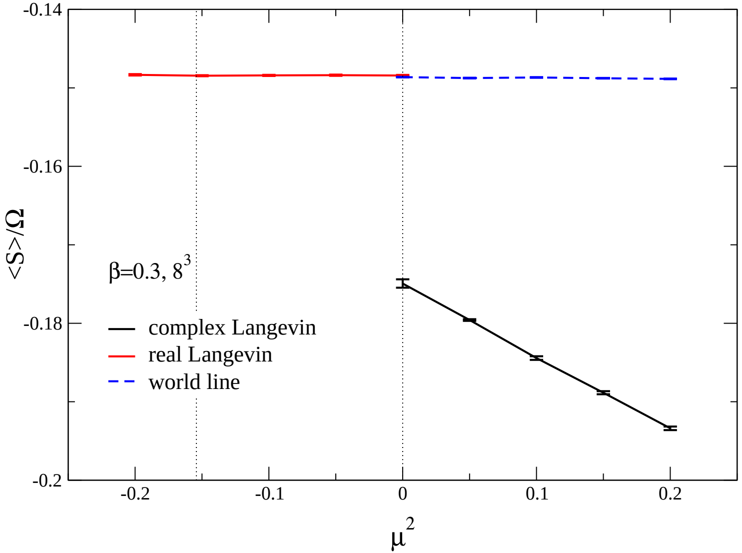
$\beta = 0.7$ ordered phase



$\beta = 0.5$ transition region



$\beta = 0.3$ disordered phase

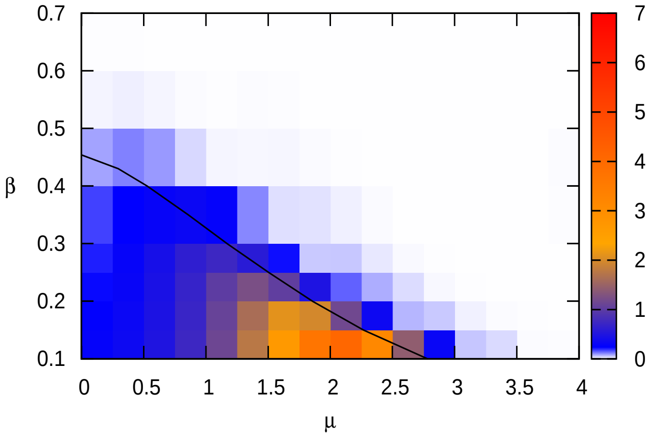


Phase diagram

- XY model at $\mu = 0$ critical coupling $\beta_c = 0.454$
- Phase transition extends into (β, μ) plane
- Strong correlation between failure and disordered phase
- Phase diagram computed using world line method
- Compute $\langle S \rangle$ using both methods over (β, μ)
- Measure ratio of action with CL and WL

$$\Delta S = \frac{S_{wl} - S_{cl}}{S_{wl}}$$

Convergence and phase diagram



Diagnostics: hot and cold starts at $\mu = 0$

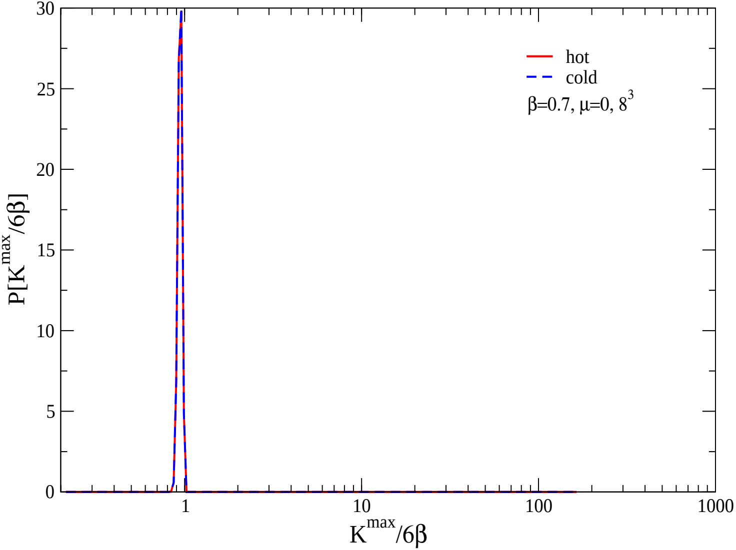
When $\mu = 0$:

- Dynamics must be different at high and low β
- Compare ensembles generated from two different initial conditions:
  - Cold start $\phi^{\mathrm{I}} = 0$ — **real dynamics**
  - Hot start ϕ^{I} random — **complex dynamics**
- Recall: $K^{\mathrm{I}} \sim \sinh(\Delta\phi^{\mathrm{I}})$ and only real noise

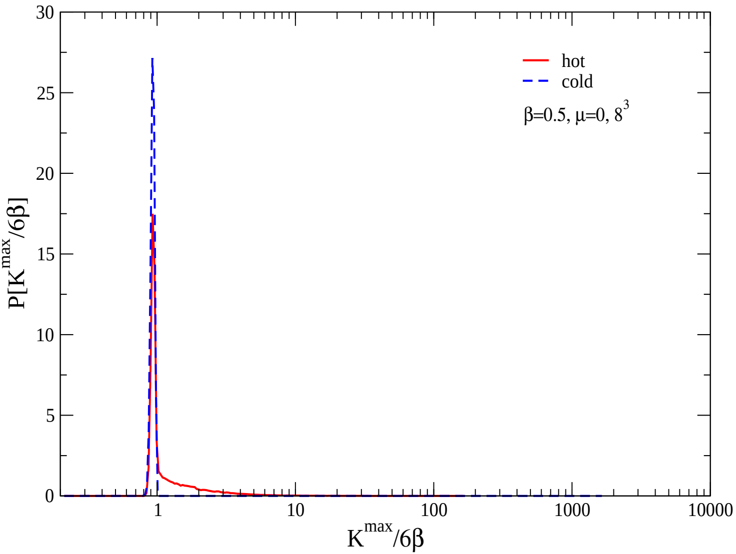
  $\Rightarrow$ Configurations with a cold start stay $\phi^{\mathrm{I}} = 0$ always
- Ensembles from a hot start lie immediately in complex plane
- *Should* converge to same result

Distribution of $K^{\max}$

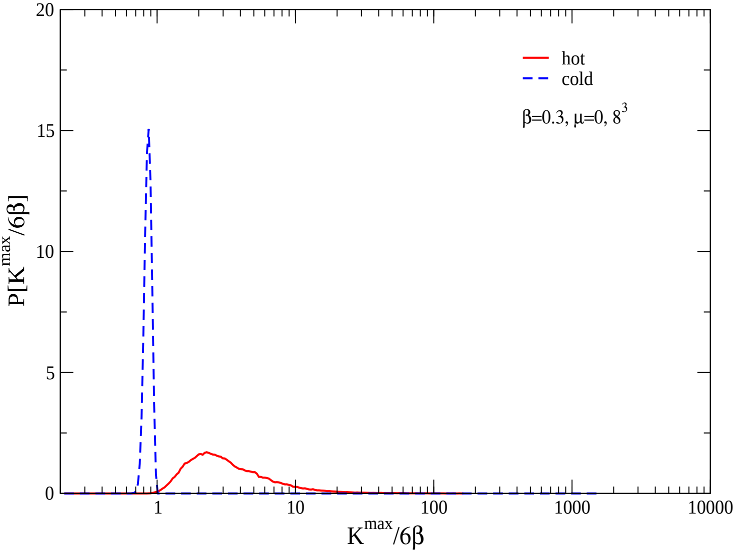
- Forces in complex dynamics not driving configuration to correct solution
- Idea: compute distribution of force terms $K^{\max}$
- Compare distribution for different β at $\mu = 0$
- Should identify differences in dynamics
- Recall: $K \leq 6\beta$ with real dynamics

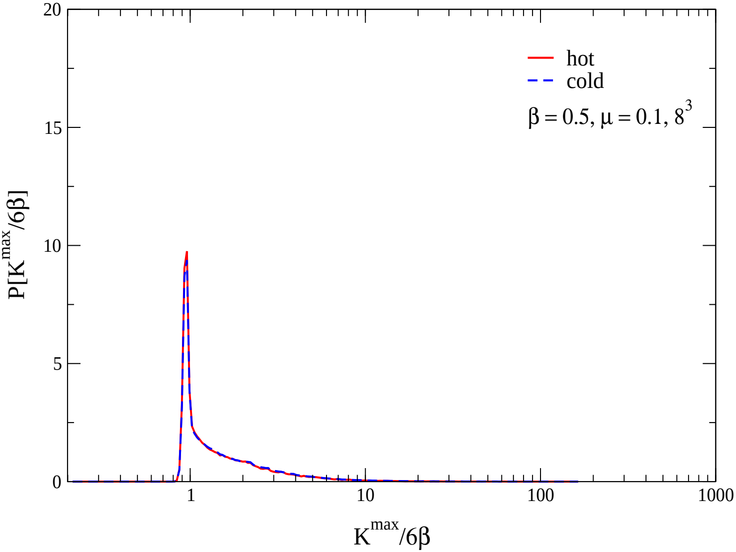


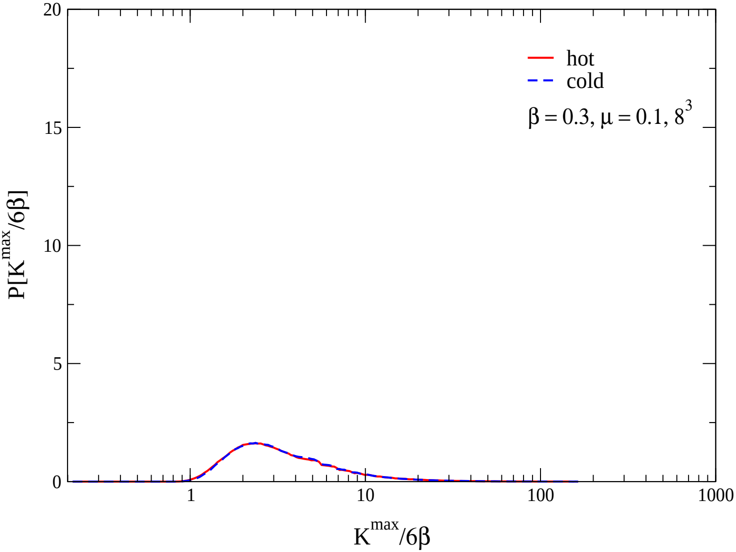
30
25
20
15
10
5
0
1
10
100
1000
$P[K^{max}/6\beta]$
$K^{max}/6\beta$
hot
cold
β=0.7, μ=0, 8^3



30
25
20
15
10
5
0
P[K^max/6β]
1
10
100
1000
10000
K^max/6β
hot
cold
β=0.5, μ=0, 8^3


hot
cold
β=0.3, μ=0, 8^3
P[K^max/6β]
K^max/6β
0
5
10
15
20
1
10
100
1000
10000


hot
cold
β = 0.5, μ = 0.1, 8^3
$P[K^{max}/6\beta]$
$K^{max}/6\beta$
0
5
10
15
20
1
10
100
1000


20
15
10
5
0
1
10
100
1000
hot
cold
β = 0.3, μ = 0.1, 8^3
P[K^max/6β]
K^max/6β

Observations of $K^{\max}$

- Crossover region $\beta \sim \beta_c$ has both types
- Correlated with phase of theory (disordered phase)
- But not with sign problem, there is no sign problem at $\mu = 0$
- Dynamics alone drive configuration to wide distribution in complex plane
- Similar effect found with studies using complex noise

Not due to sign problem

Conclusion/Outlook

- Two old problems encountered
- Runaways eliminated with adaptive stepsize
- Greater insight into incorrect convergence from $\mu = 0$ hot/cold starts
- Problem is subtle, depends on phase of theory
- Caused by dynamics not driving to correct configuation
- Similar features to other simple models using complex noise

But not caused by sign problem