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Thermodynamic Diagnostics for **Complex Langevin Simulations:**

The Role of Configurational Temperature

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based on: *arXiv:2509.08287 [hep-lat]*
arXiv:2509.13314 [hep-lat]

PLAN OF TALK

1. Complex Langevin Method (CLM)
2. Challenges and Reliability of CLM
3. Configuration-Based Thermometer: Thermodynamic Diagnostics
4. Configurational Temperature: Reliability criteria in CLM
   — 1D PT-Symmetric Model
   — 3D XY Model

Complex Langevin for Complex Actions

why complex Langevin ?

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\phi \; \mathcal{O}(\phi) \; e^{-S_E} \longrightarrow \boxed{\textit{generate } \{\phi_i\} \textit{ with probability } e^{-S[\phi_i]}}$$

In Path Integral Monte Carlo

$$\langle \mathcal{O} \rangle = \frac{1}{N} \sum_{i=1}^{N} \mathcal{O}(\phi_i)$$

For Complex Actions

$$\boxed{e^{-(S_{re} + iS_{im})} \rightarrow \cancel{\text{probability weight}}}$$

$S = S_{real} + iS_{imag}$ such that $e^{-S} \equiv |e^{-S}| e^{i\theta}$

eg. $\det(M) \equiv |\det M| e^{i\theta}$, $\beta \equiv \beta_r e^{i\theta}$, θ-*term*…

sign-problem in Monte Carlo: complex-phase/complex-action problem.

Complex Langevin for Complex Actions

why complex Langevin ?

In QCD Phase Diagram

exploring phase structure under control parameters

external EM fields ■ *complex actions!*

temperature T, μ_{B}, μ_{I}, eB, E, Ω, a …

chemical potentials *boosts and rotations, acceleration etc.*

hinder direct estimation of physical aspects like CEP…

Real Langevin Method

Parisi and Wu (1981)

- First investigated in context of field theories by Parisi and Wu in 1981
- Stochastic evolution of fields along the fictitious time, Langevin time (τ; $\sim$ MC time)
- Langevin equation: Consider 0-d theory: real action $S[\phi]$ and scalar field ϕ

$$\boxed{\partial_\tau \phi(\tau) = v(\phi, \tau) + \eta(\tau)}$$

analogy with Brownian motion

SDE Stochastic Differential Equation

drift (friction/gradient descent/dissipation)

$$v(\phi, \tau) = -\frac{\delta S[\phi]}{\delta \phi(\tau)}$$

noise (kick/diffusion)

$$\langle \eta(\tau) \rangle = 0$$

$$\langle \eta(\tau)\eta(\tau') \rangle = 2\,\delta(\tau - \tau')$$

FDT

Fluctuation-Dissipation

- Gaussian noise encodes the quantum fluctuations around the classical drift part

Real Langevin Method

Parisi and Wu (1981)

Stochastic Quantization

expectation values $\leftrightarrow$ equilibrium values

$\partial_\tau \phi(\tau) = v(\phi, \tau) + \eta(\tau)$

SDE $\leftrightarrow$ FPE

$$\langle \mathcal{O}(\phi) \rangle_\rho = \int d\phi \ \rho(\phi) \mathcal{O}(\phi)$$

$$\langle \mathcal{O}(\phi, \tau) \rangle_P = \int d\phi \ P(\phi, \tau) \mathcal{O}(\phi)$$

where $\rho(\phi)$ is Boltzmann weight

$$\rho(\phi) = e^{-S[\phi]}$$

where $P(\phi, \tau)$ evolves Fokker Planck Eq. **FPE**

$$\frac{\partial P[\phi, \tau]}{\partial \tau} = \underbrace{\frac{\delta}{\delta \phi(\tau)} \left(\frac{\delta}{\delta \phi(\tau)} + \frac{\delta S[\phi]}{\delta \phi(\tau)} \right)}_{\mathscr{L}^T \text{ : Langevin operator}} P[\phi, \tau]$$

$$\lim_{\tau \to \infty} \langle \mathcal{O}(\phi; \tau) \rangle_{P(\phi;\tau)} \simeq \langle \mathcal{O}(\phi) \rangle_\rho \quad \leftrightarrow \quad \lim_{\tau \to \infty} P(\phi, \tau) \simeq \rho(\phi) = e^{-S[\phi]}$$

Complex Langevin Method

Klauder (1983), Parisi (1983)

- A formal extension of real Langevin, independently by Parisi and Klauder

$$\phi \to \Phi = \phi_x + i\phi_y$$

$$\mathcal{O}(\phi) \to \mathcal{O}(\Phi) = \mathcal{O}(\phi_x + i\phi_y)$$

- Complex Langevin evolution: Consider 0-d theory with complex action $S[\Phi]$

$$\frac{\partial \phi_x}{\partial \tau} = -\,\mathrm{Re}\left(\frac{\delta S[\Phi]}{\delta \Phi}\right) + \eta_R(\tau) \qquad \frac{\partial \phi_y}{\partial \tau} = -\,\mathrm{Im}\left(\frac{\delta S[\Phi]}{\delta \Phi}\right)$$

$$\Longrightarrow \boxed{\partial_\tau \Phi(\tau) = v(\Phi,\tau) + \eta(\tau)}$$

Complex Langevin Method in a nutshell

Complex extension of Stochastic Quantization

expectation values ↔ equilibrium values

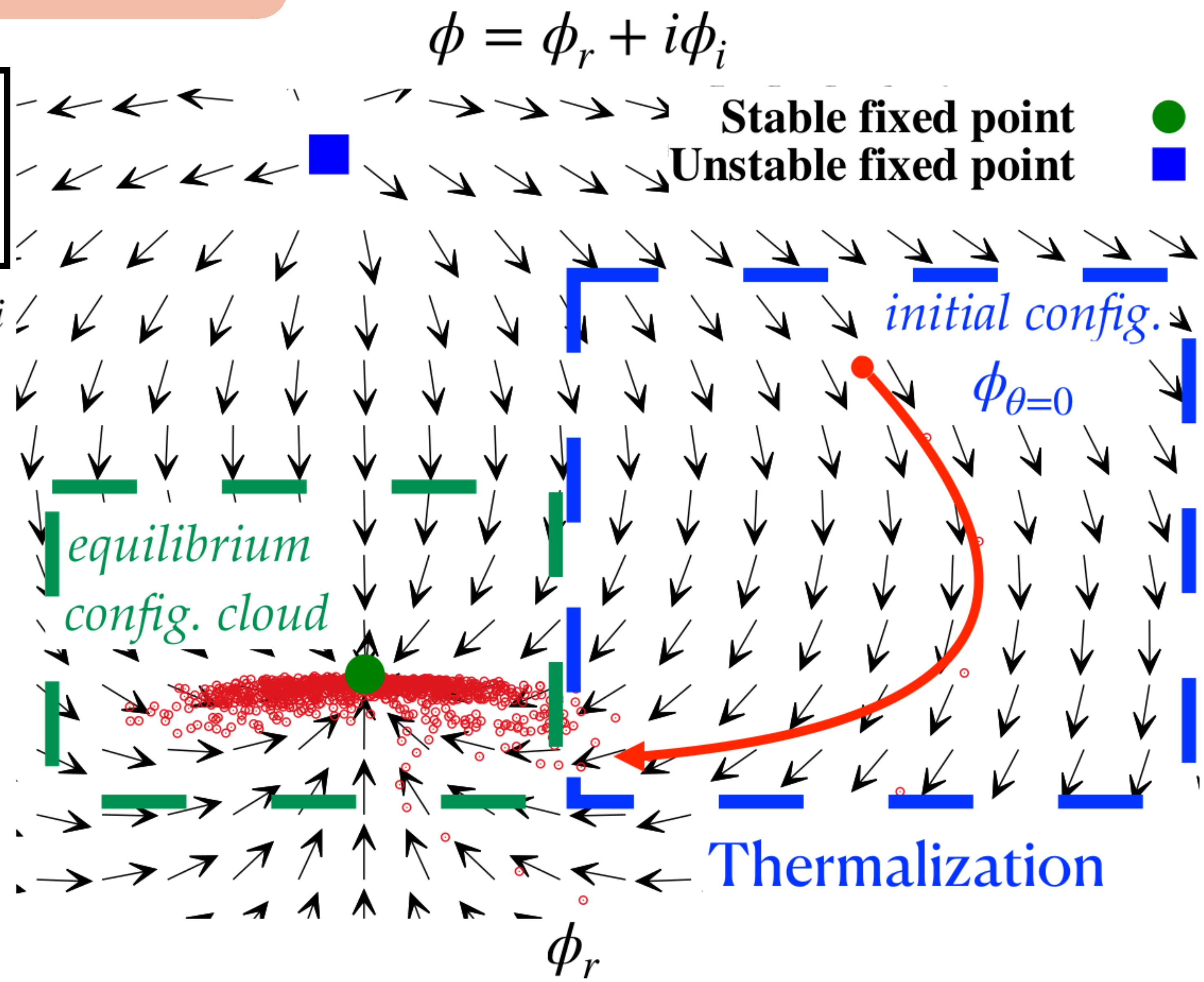
Klauder (1983), Parisi (1983)

$$\boxed{\partial_\tau \Phi(\tau) = v(\Phi, \tau) + \eta(\tau)}$$

In simulations Discretized Eq.

$\Delta\tau \to \epsilon$; *small* ϵ, $O(\epsilon)$

$$\Phi_{n+1} \leftarrow \Phi_n = \epsilon\, v(\Phi, \tau) \; + \; \sqrt{\epsilon}\; \eta(\tau)$$



Complex Langevin Method in a nutshell

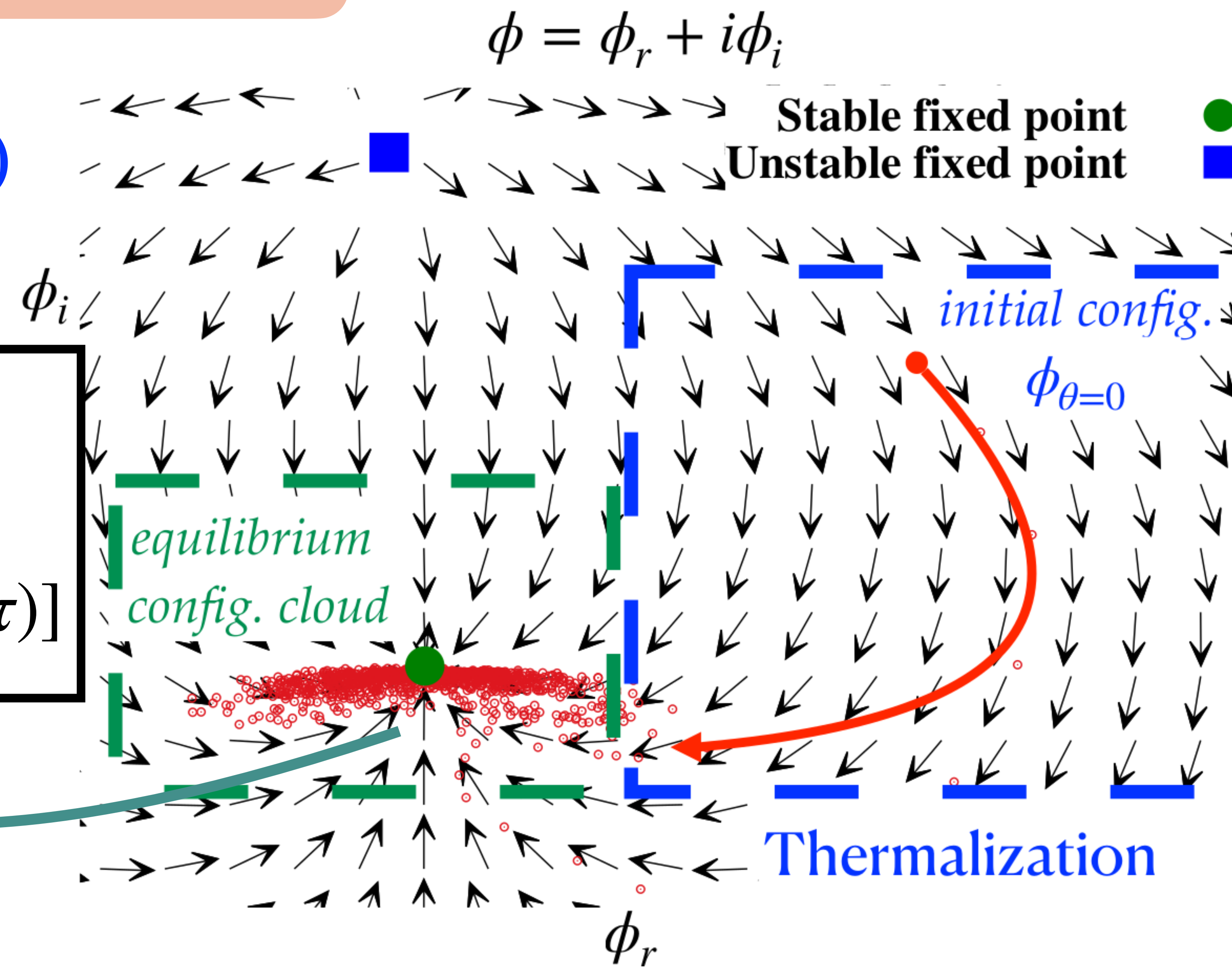
Complex extension of Stochastic Quantization

expectation values ↔ equilibrium values

Klauder (1983), Parisi (1983)

$$\partial_\tau \Phi(\tau) = v(\Phi, \tau) + \eta(\tau)$$

$$\langle \mathcal{O}[\Phi(\tau)] \rangle_P = \int d\phi_x d\phi_y \times P[\phi_x, \phi_y; \tau]\, \mathcal{O}[\Phi(\tau)]$$



Complex Langevin Method
Correct Convergence

Klauder (1983), Parisi (1983)

- Expectation values of holomorphic observables $\mathcal{O}$ in real and complex configuration space

$$\langle \mathcal{O}(\Phi) \rangle_{P(\tau)} = \frac{\int d\phi_x d\phi_y \; P(\phi_x, \phi_y; \tau) \; \mathcal{O}(\phi_x + i\phi_y)}{\int d\phi_x d\phi_y \; P(\phi_x, \phi_y; \tau)}$$

$$\langle \mathcal{O}(\phi) \rangle_{\rho(\tau)} = \frac{\int d\phi \; \rho(\phi; \tau) \; \mathcal{O}(\phi)}{\int d\phi \; \rho(\phi; \tau)}$$

- Complex Langevin is justified if

$$\boxed{\lim_{\tau \to \infty} \langle \mathcal{O} \rangle_{P(\tau)} \overset{?}{\simeq} \langle \mathcal{O} \rangle_{\rho(\tau)}}$$

When action is complex,
no such proof of convergence exists!

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Reliability of CLM

$$\lim_{\tau\to\infty} \boxed{\langle \mathcal{O} \rangle_{P(\tau)}} \overset{?}{\simeq} \boxed{\langle \mathcal{O} \rangle_{\rho(\tau)}}$$

Caveats in convergence of complex Langevin (challenging to find eq. solutions)

No (even worse incorrect) convergence

Challenges: Excursion Problem

- In Langevin evolution excursion in imaginary direction or large drift
- Gauge theories: matrices X_μ too far away from Hermitian $\mathrm{SU}(N) \to \mathrm{SL}(N, \mathbb{C})$
- Possible stabilization techniques:

Adaptive stepsize

Aarts, James, Seiler, and Stamatescu (2009)

$$\epsilon = \frac{\gamma}{K_{\max}(\theta)}$$

say $O(\epsilon^2)$, mitigates discretization instabilities

Dynamical stabilization

Attanasio and Jäger (2019)

Gauge cooling

Seiler, Sexty and Stamatescu (2012)

$$X_\mu \to X'_\mu = g X_\mu g^{-1} \text{ where } g \in \mathrm{SL}(N, \mathbb{C})$$

$$\mathcal{N}_H = -\frac{1}{10N} \sum_{\mu=1}^{10} \mathrm{Tr}\left[\left(X_\mu - X_\mu^\dagger\right)^2\right]$$

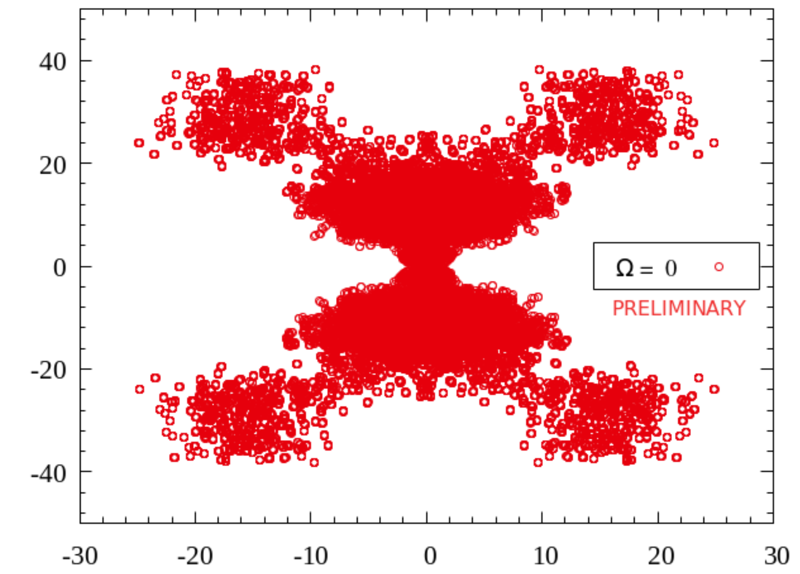
Nagata, Nishimura and Shimasaki (2016)

Norm $\mathcal{N}_H$ not invariant under the extra symmetry so minimize

Challenges: Singular Drift

- Fermion operator $\mathscr{M}$ has near-zero eigenvalues $(\det[\mathscr{M}] \sim 0)$
- The drift term diverges: results unreliable

$$\frac{\partial S_{\mathrm{f}}}{\partial (X_\mu)_{ji}} = -\frac{1}{2}\mathrm{Tr}\left(\frac{\partial \mathscr{M}}{\partial (X_\mu)_{ji}} \boxed{\mathscr{M}^{-1}}\right)$$



- Possible solutions:

Mass deformations

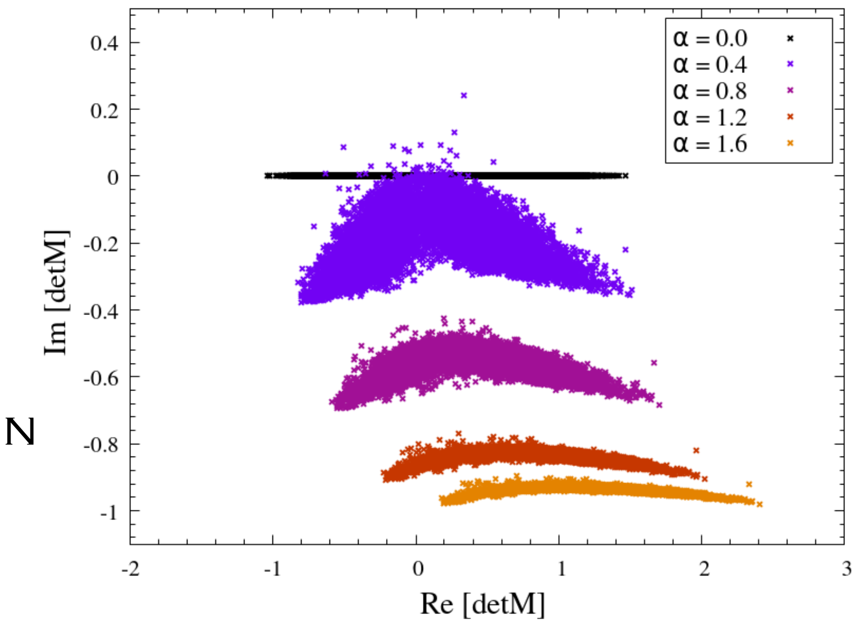
$$S \leftarrow S + \Delta S$$

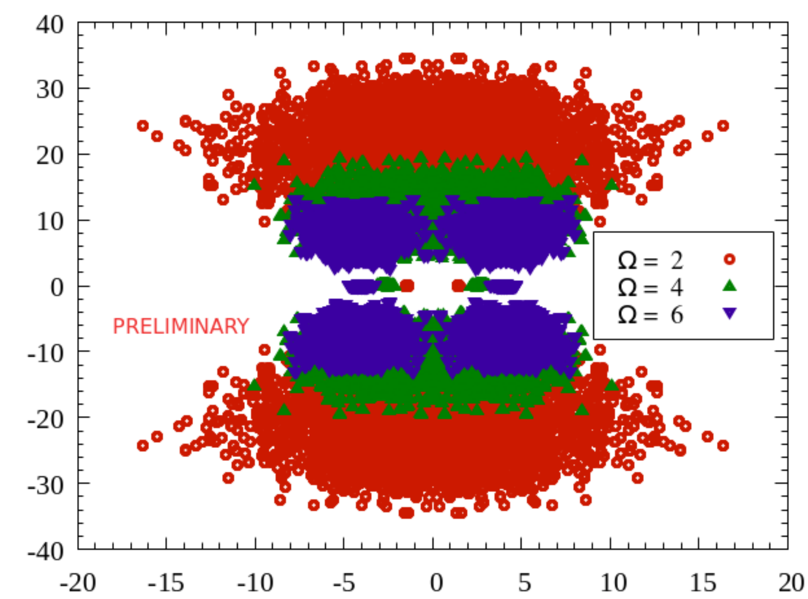
Ito and Nishimura (2016)

Twisted boundary condition

$$\psi\left(t+\beta\right) = e^{i\alpha}\psi\left(t\right)$$

Joseph and Kumar (2021)





Reliability Criteria

When action is complex, no exact proof of convergence exists!

need reliability/correctness criteria

$$\langle \mathscr{L}^T \mathscr{O} \rangle = 0$$

$\mathscr{L}$: Langevin operator in **FPE**

$$\frac{\partial P[\phi_x, \phi_y; \theta]}{\partial \theta} = \mathscr{L}^T P[\phi_x, \phi_y; \theta]$$

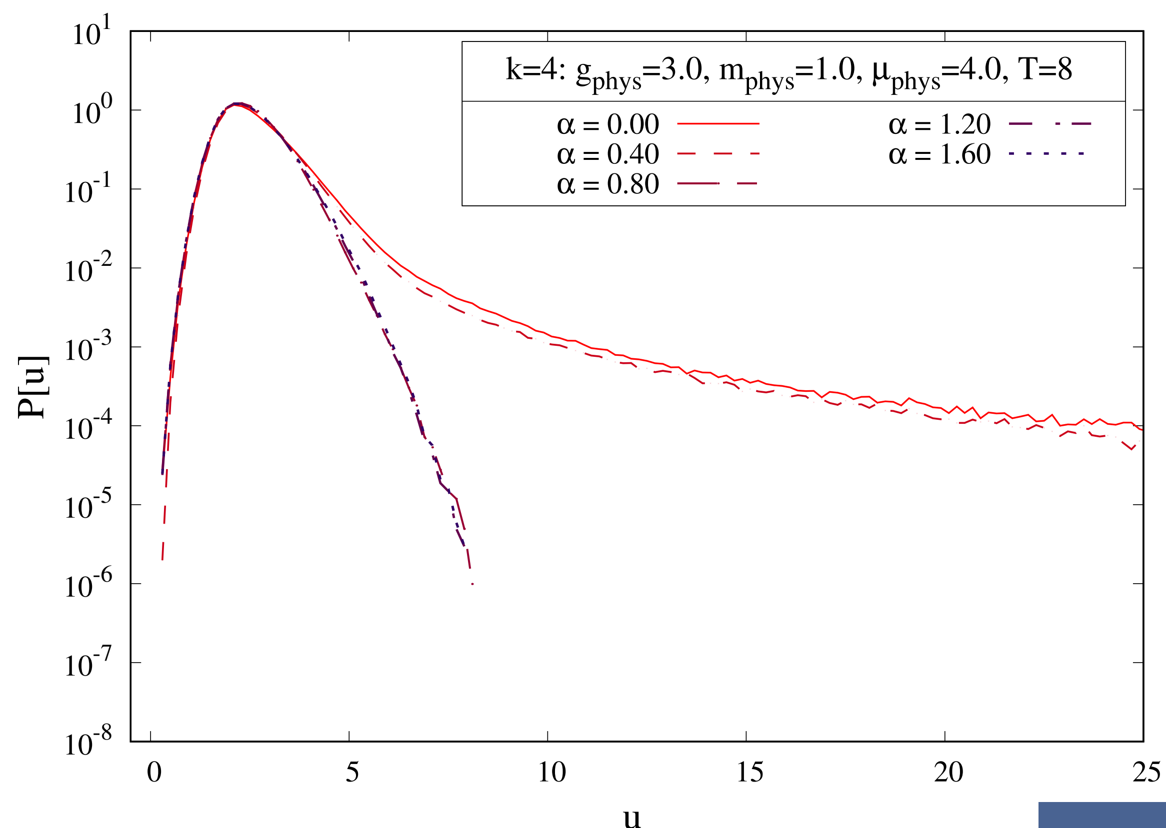
Aarts, Seiler, and Stamatescu (2009)

$$u = \left| \frac{\partial S[\Phi]}{\partial \Phi} \right|$$

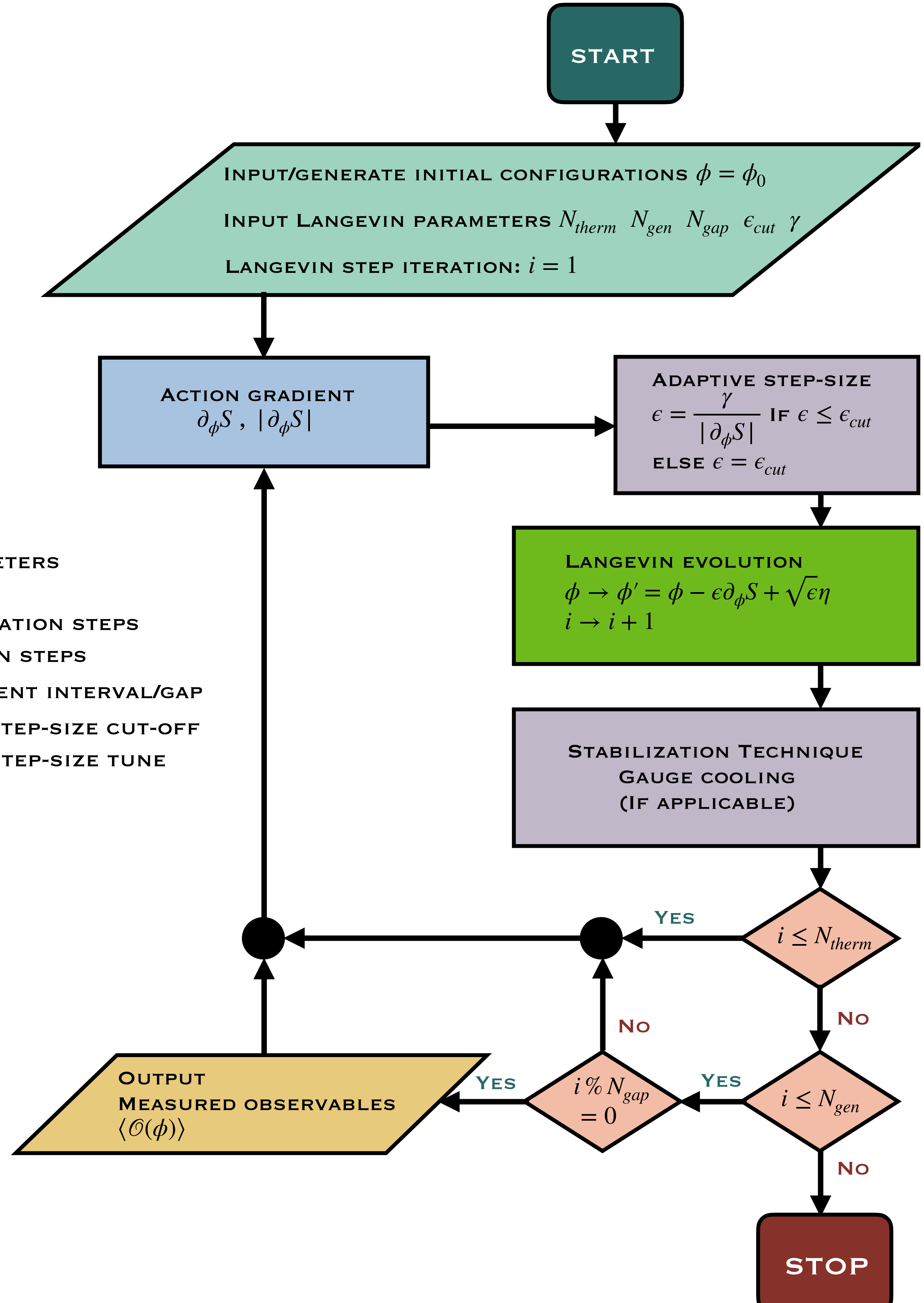
u : magnitude of drift

Nagata, Nishimura, and Shimasaki (2016)

Probability distribution $P(u)$ falls off exponentially or faster



CLM Flowchart



Langevin parameters

N_{therm}: Thermalization steps
N_{gen} : Generation steps
N_{gap} : Measurement interval/gap
ϵ_{cut} : Langevin step-size cut-off
γ : Langevin step-size tune

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Configuration-Based Thermometer

$$\boxed{\beta = (k_B T)^{-1} \equiv \left(\frac{\partial S}{\partial E}\right)\Big|_V}$$

Thermodynamical relation among energy-related observables $P, E, S, N, \ldots \equiv f(T, V, \mu, eB \ldots)$

Isochoric transformations : $dE = T\, dS - P\, dV$

Change in entropy under infinitesimal energy shift at fixed volume!

displacement in phase-space

$$\Delta S,\ \Delta E\ \leftarrow \delta\Gamma : \Gamma' - \Gamma$$

$$S(E) = k_B\ \ln \Omega_{\Gamma(E,\,V,\,N)} \equiv k_B\ \ln\left(\int_{C(E)} d\Gamma\right)$$

$$C(E) \equiv \{\Gamma\,|\,H(\Gamma) \leq E\}$$

$$\Gamma \equiv \{q_1, q_2, \cdots, q_N;\ p_1, p_2, \cdots, p_N\}$$

Configurations and momentum phase space

Micro-canonical Ensemble $E, S, N, \ldots$

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Dynamical Approach to Temperature

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(Received 17 May 1996)

We present a new dynamical approach for measuring the temperature of a Hamiltonian dynamical systems in the microcanonical ensemble of thermodynamics. We show that under the hypothesis of ergodicity the temperature can be computed as a time average of the functional, $\nabla \cdot (\nabla H/\|\nabla H\|^2)$, on the energy surface. Our method not only yields an efficient computational approach for determining the temperature, it also provides an intrinsic link between dynamical systems theory and the statistical mechanics of Hamiltonian systems. [S0031-9007(96)02078-9]

PACS numbers: 05.20.Gg, 02.40.Vh, 05.20.–y, 05.70.–a

Rugh, PRL (1997)

Configuration-Based Thermometer

$$\beta = (k_B T)^{-1} \equiv \left(\frac{\partial S}{\partial E}\right)\Bigg|_V$$

Change in entropy under infinitesimal energy shift at fixed volume!

$$\boxed{\begin{array}{c} \Gamma' \leftarrow \Gamma + \Delta E\ n(\Gamma) \\ \text{yields} \\ H(\Gamma') - H(\Gamma) \equiv \Delta E \end{array}}$$

Rugh, PRL (1997)

Displacements in Configuration!

$H(q, p)$: separable $\{q,\ p\}$ theories

$$H(\Gamma),\ \Delta S,\ \Delta E\ \leftarrow \delta\Gamma : \delta q,\ q'$$

$$q' \equiv \{q_1', q_2',\ \cdots, q_N'\}$$

$$\vec{n}(\vec{\Gamma}) \equiv \vec{n}(\vec{q}) = \frac{\vec{\nabla}_{\vec{q}} H}{\vec{\nabla}_{\vec{q}} H \cdot \vec{\nabla}_{\vec{q}} H},$$

only configurational components such that

$$\vec{\nabla}_{\vec{q}} \equiv \left(\frac{\partial}{\partial \vec{q}_1},\ \cdots,\ \frac{\partial}{\partial \vec{q}_N}\right)$$

Configuration-Based Thermometer

$$\beta = (k_B T)^{-1} \equiv \left(\frac{\partial S}{\partial E}\right)\bigg|_V$$

$$\Delta S \simeq k_B \Delta E\, \vec{\nabla}_{\vec{q}} \cdot \vec{n}(\vec{q}), \quad \xrightarrow{\Delta E \to 0} \quad \beta = (k_B T)^{-1} \equiv \left\langle \vec{\nabla}_{\vec{q}} \cdot \frac{\vec{\nabla}_{\vec{q}} \Phi}{|\vec{\nabla}_{\vec{q}} \Phi|^2} \right\rangle$$

For $H(q) \equiv V(q)$;

$$\underset{\text{drift}}{\vec{g}} = \vec{\nabla}_{\vec{q}} V, \qquad \overset{\text{hessian}}{\mathbb{H}} = \vec{\nabla}_{\vec{q}} \vec{\nabla}_{\vec{q}}^T V.$$

$$\boxed{\beta = (k_B T)^{-1} \equiv \vec{\nabla}_{\vec{q}} \cdot \left(\frac{\vec{g}}{|\vec{g}|^2}\right) = \overbrace{\frac{\mathrm{Tr}(\mathbb{H})}{|\vec{g}|^2} - 2\frac{\vec{g}^T \mathbb{H} \vec{g}}{|\vec{g}|^4}}^{\beta_{config}}}$$

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1D PT-symmetric Theory Recipe

$$V_\delta(\phi) = -\frac{g}{2+\delta}(ig)^{2+\delta}\ ; \quad g, \delta > 0$$

scalar field theory with PT-symmetry
non-Hermitian posses real, positive-definite spectra

Bernard, Savage (2001)
Guralnik, Pehlevan (2007)

$$S_\delta^E = \int_0^\beta d\tau \left[\frac{1}{2}(\partial_\tau \phi)^2 + V_\delta(\phi)\right]$$

Euclidean time τ compactified to circumference of thermal circle

$$\beta \equiv 1/(k_B T)$$

$$S_{\delta,\,L}^E \equiv \sum_{n=0}^{N_\tau - 1}\left[\frac{(\phi_{n+1}-\phi_n)^2}{2} - \frac{g}{2+\delta}(i\phi_n)^{2+\delta}\right]$$

dimensionless field and coupling:

$$\phi = \phi_{\mathrm{phys}}/\sqrt{a}, \quad g = a^{2+\delta/2} g_{\mathrm{phys}}$$

…. simulate using CLM

Applying CLM to PT-symmetric Theory

$$G_k \equiv \langle \phi^k \rangle; \;\; k \in Z$$

equal-time correlation functions

parameters:

$\delta = 1, 2$

$g = 1$

$\boxed{\beta = 1}$

$N_\tau = 128$

$\phi_{start} = 0.0 - i1.0$

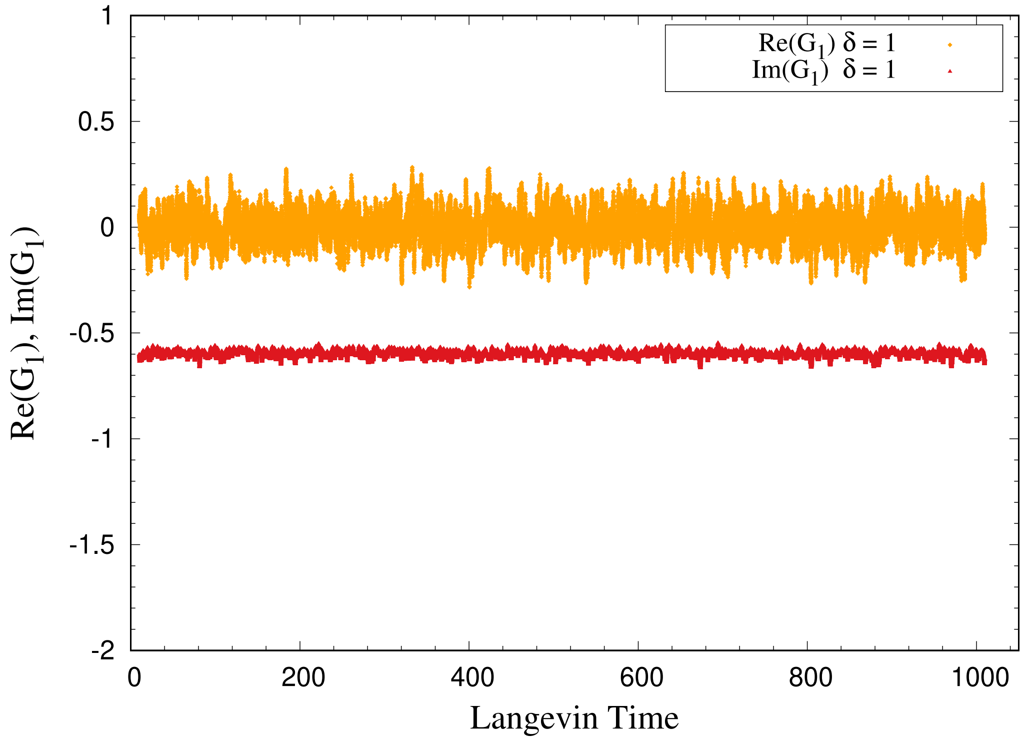
hyperparameters:

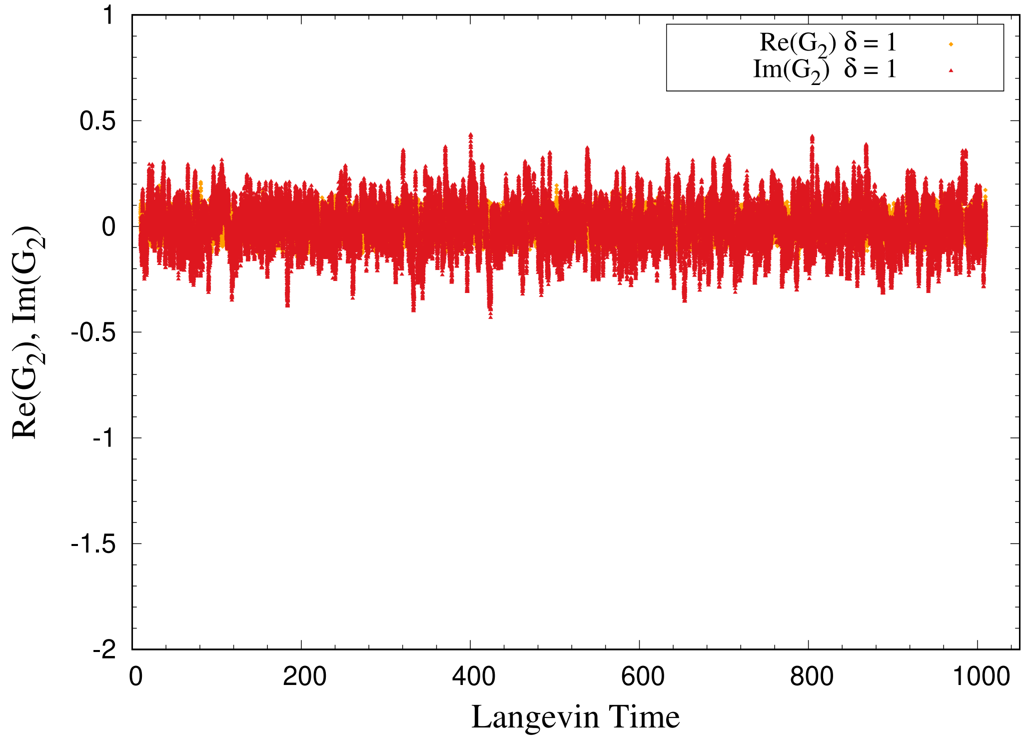
$N_{therm} = 10^4$

$N_{gen} = 10^6$

$\text{gap} = 10$

$\epsilon_{\text{adap}} \leq 10^{-3}$





Configurational Temperature of CL trajectories

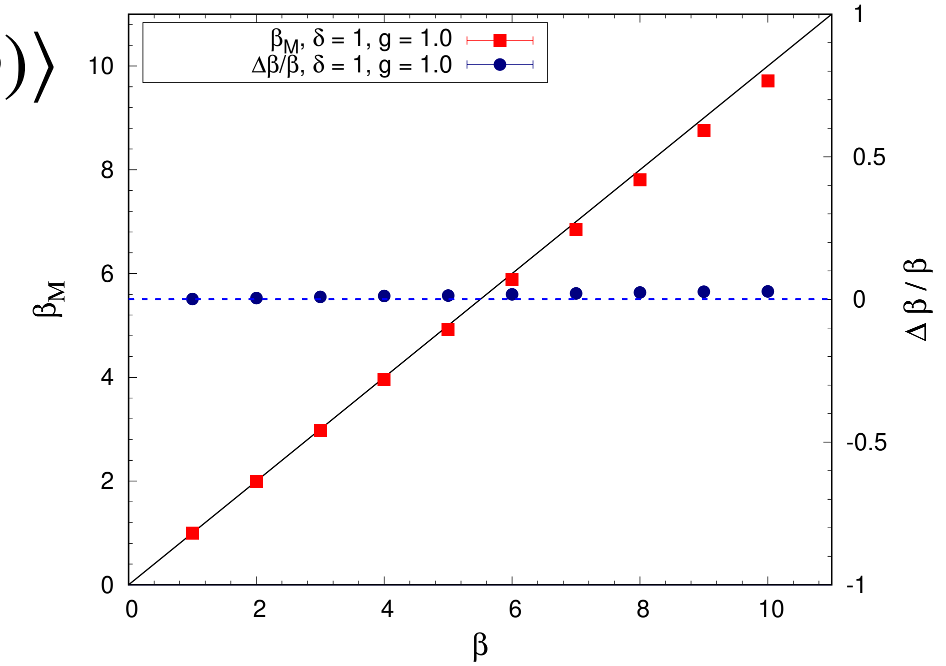
$$\beta_M \equiv \langle \beta_{config}(\phi) \rangle$$

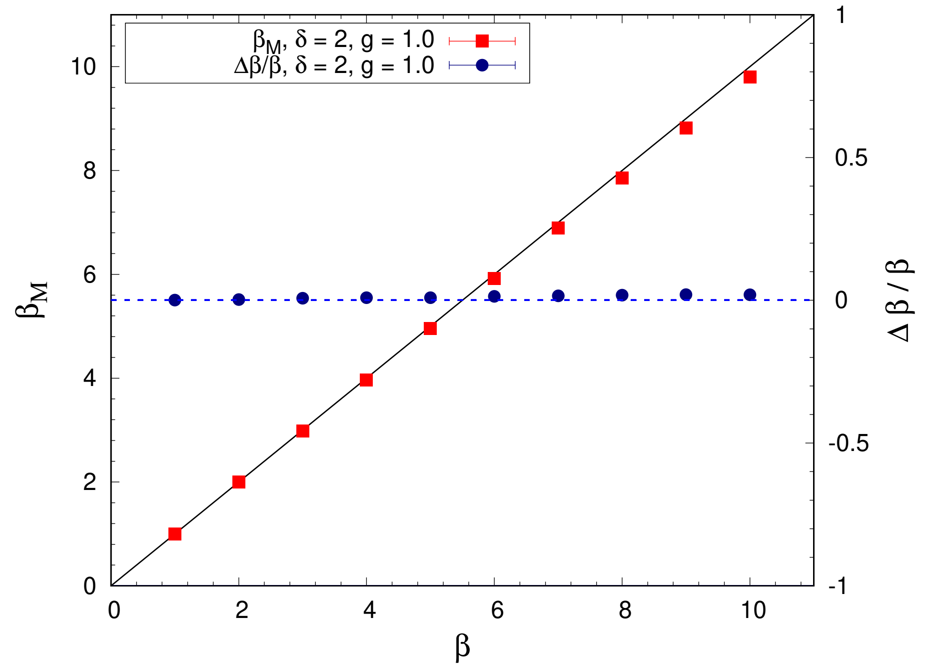
$$\boxed{\beta_{config}(\phi) \equiv \frac{\mathrm{Tr}(\mathbb{H})}{|\vec{g}|^2} - 2\frac{\vec{g}^T \mathbb{H} \vec{g}}{|\vec{g}|^4}}$$

$$\mathrm{Tr}(\mathbb{H}) \equiv \sum_n h_{nn}$$

$$|\vec{g}|^2 \equiv \sum_n g_n^2$$

$$g_n = \frac{1}{\beta}\frac{\partial S}{\partial \phi_n}, \qquad h_{nm} = \frac{1}{\beta}\frac{\partial^2 S}{\partial \phi_n \partial \phi_m}.$$



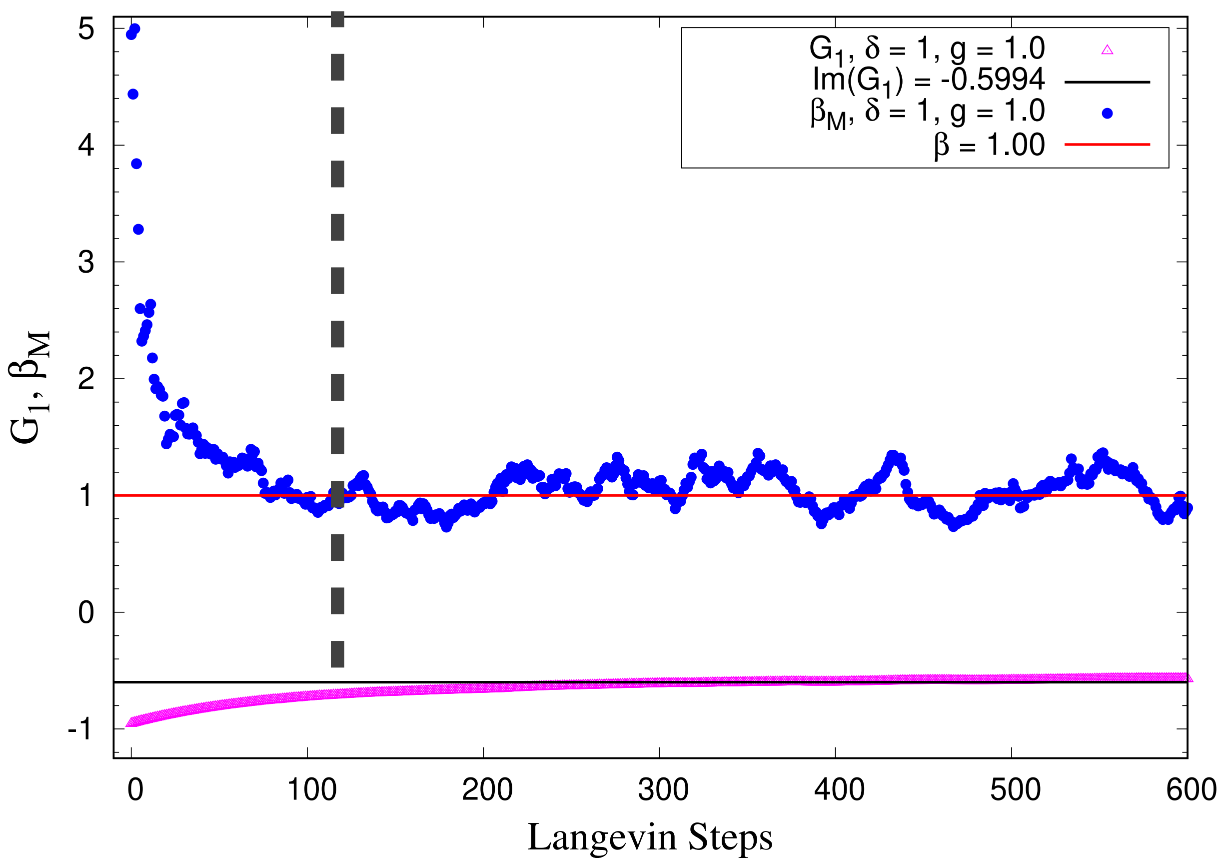


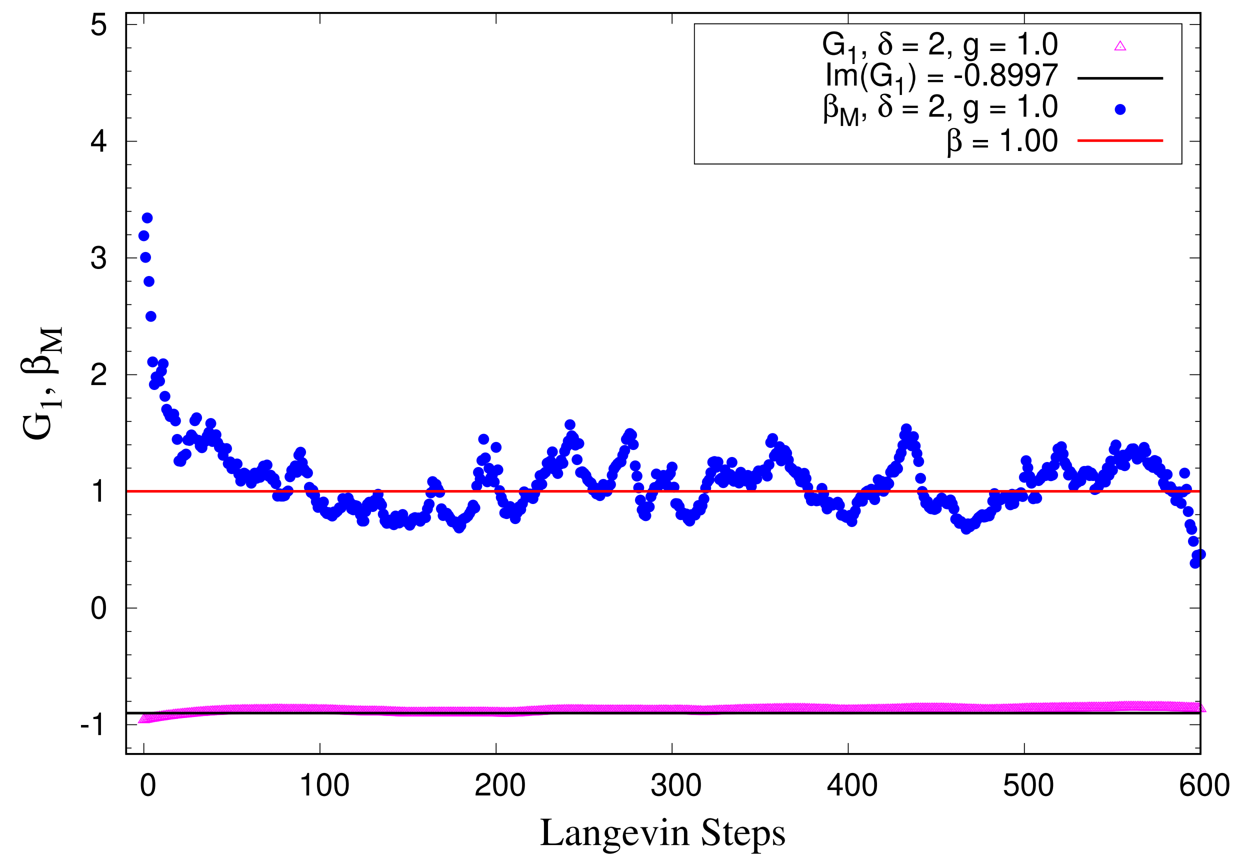
Configuration-Based Thermometer: Reliability Criteria in CLM

Can it detect incorrect convergence of complex Langevin!

- Monitoring thermalization
- Assessing Langevin step size dependence
- Detecting algorithmic errors: validating strength of drift and noise

Configurational Temperature For
A. Monitoring thermalization





Configurational Temperature for B. Assessing Langevin Step-Size

β	ϵ	$\beta_M(\delta = 1)$	$\beta_M(\delta = 2)$
1.00	0.0001	$1.0002(15) - i0.0105(7)$	$0.9845(22) - i0.0206(23)$
	0.001	$0.9983(15) - i0.0027(7)$	$0.9995(22) - i0.0078(21)$
	0.01	$0.9830(15) - i0.0010(7)$	$0.9898(23) - i0.0008(22)$
	0.03	$0.9474(14) - i0.0006(7)$	$0.9663(29) - i0.0016(28)$
	0.1	$0.8251(12) - i0.0000(7)$	–
	0.2	$0.6437(11) - i0.0010(8)$	–

Correct convergence also subject to:

Large Langevin time; $\tau \to \infty$

Small stepsize; $\epsilon \to 0$

Estimate sufficiently small stepsize; possibility of better sensitivity than drift based adaptive stepsize

Configurational Temperature for C. Detecting Algorithmic Errors

Algorithmic error into the noise normalization of the discretized Langevin equation.

Replace the correct Gaussian correlation:

$$\langle \eta(\theta)\eta(\theta') \rangle = 2\,\delta_{\theta\theta'}$$

$$\downarrow$$

$$\langle \eta(\theta)\eta(\theta') \rangle = \sigma\,\delta_{\theta\theta'}$$

$\sigma > 0,\ \sigma \neq 2$

mis-scaling

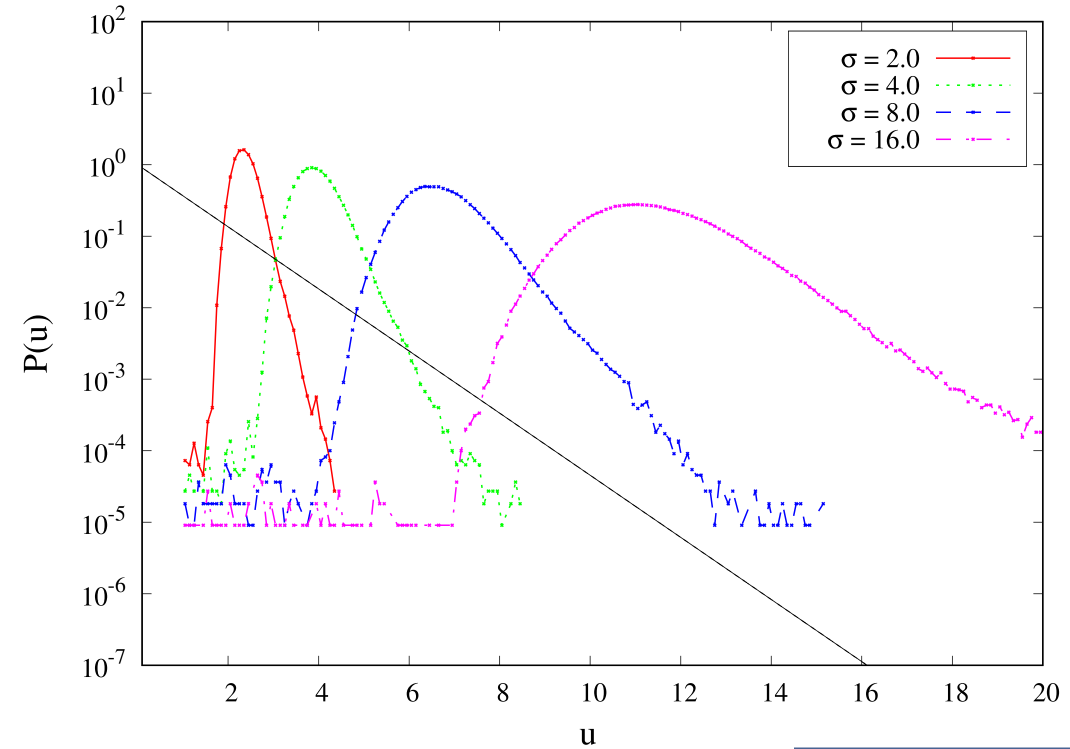
β	σ	$\beta_M(\delta = 1)$	$\beta_M(\delta = 2)$
1.00	0.5	$3.9888(59) - i0.0070(18)$	$3.9941(64) - i0.0094(40)$
	1.0	$1.9953(29) - i0.0045(11)$	$1.9980(36) - i0.0116(29)$
	2.0	$0.9983(15) - i0.0027(7)$	$0.9994(22) - i0.0078(21)$
	4.0	$0.4996(7) - i0.0015(4)$	$0.4986(14) - i0.0011(14)$

Effectively validates the balance between of drift and noise

Reliability Criteria Comparison

δ	β	σ	Criterion 1 $\beta_M = \beta$	Criterion 2 $\langle LG_1 \rangle = 0$	Criterion 3 Drift term fall-off
1.0	1.0	2.0	$0.9968(5) + i\,0.0000(2)$ (Satisfied)	$-0.0010(3) - i\,0.0000(1)$ (Satisfied)	Exponential (Satisfied)
		4.0	$0.4984(2) + i\,0.0000(1)$ (Not Satisfied)	$-0.0014(5) - i\,0.0000(2)$ (Satisfied)	Exponential (Satisfied)
		8.0	$0.2492(1) + i\,0.0000(0)$ (Not Satisfied)	$-0.0019(9) - i\,0.0000(4)$ (Satisfied)	Exponential (Satisfied)
		16.0	$0.1246(0) + i\,0.0000(0)$ (Not Satisfied)	$-0.0027(14) - i\,0.0000(6)$ (Satisfied)	Exponential (Satisfied)
2.0	1.0	2.0	$0.9972(7) + i\,0.0005(6)$ (Satisfied)	$-0.0010(5) - i\,0.0000(3)$ (Satisfied)	Exponential (Satisfied)
		4.0	$0.4975(12) + i\,0.0013(6)$ (Not Satisfied)	$-0.0013(8) - i\,0.0000(6)$ (Satisfied)	Exponential (Satisfied)
		8.0	$0.2485(3) + i\,0.0004(3)$ (Not Satisfied)	$-0.0018(15) - i\,0.0000(10)$ (Satisfied)	Exponential (Satisfied)
		16.0	$0.1238(2) + i\,0.0002(3)$ (Not Satisfied)	$-0.0023(25) - i\,0.0000(18)$ (Satisfied)	Non-exponential (Not Satisfied)

- *Criterion 1* highly sensitive , reflects all noise normalization deviations immediately as $\beta_M \neq \beta$
- *Criterion 2* fails to flag algorithmic errors
- *Criterion 3* delayed sensitivity



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3D XY Model Brief Recipe

angular variables $0 \leq \phi_x < 2\pi$

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

temporal $\nu = 0$

spatial $\nu = 1,2$

lives on a 3d lattice $\Omega = N_\tau N_\sigma^2$

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

coupling / interaction strength

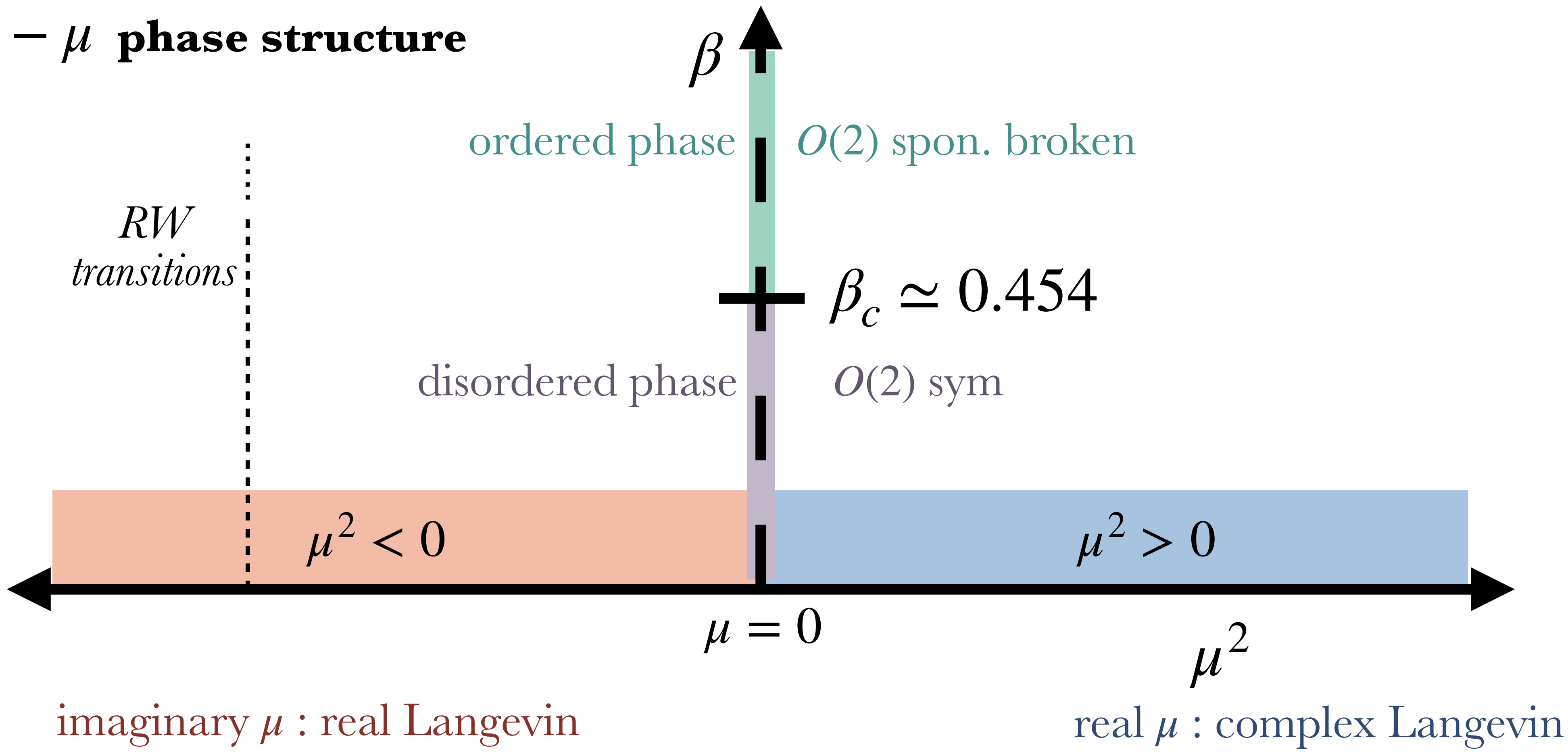
chemical potential μ *couples to conserved charged* $O(2)$

$\phi_x \to \phi_x + \alpha$

3D XY Model Brief Recipe

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

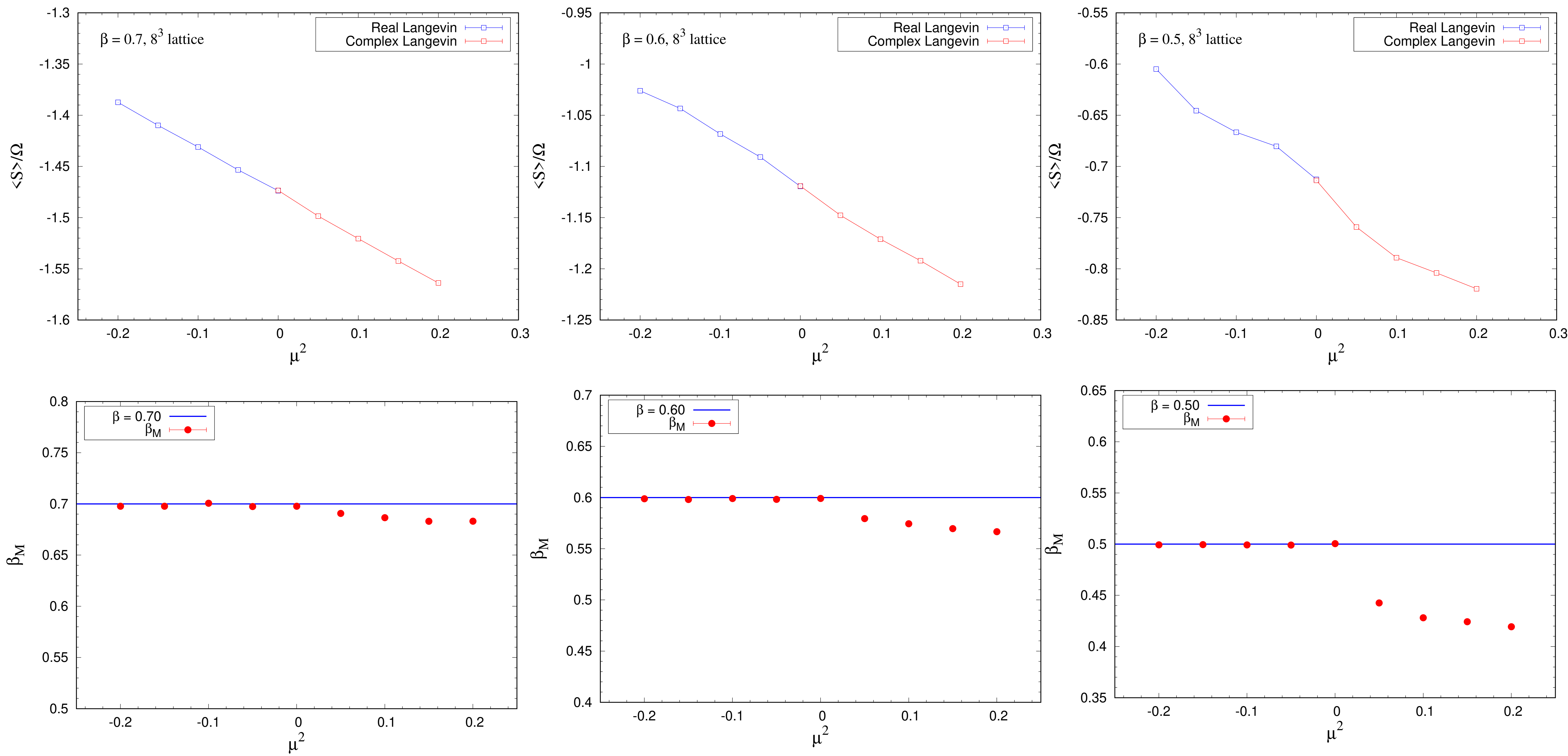
rich $\beta - \mu$ phase structure



Can configurational β-estimator address reliability of complex Langevin?

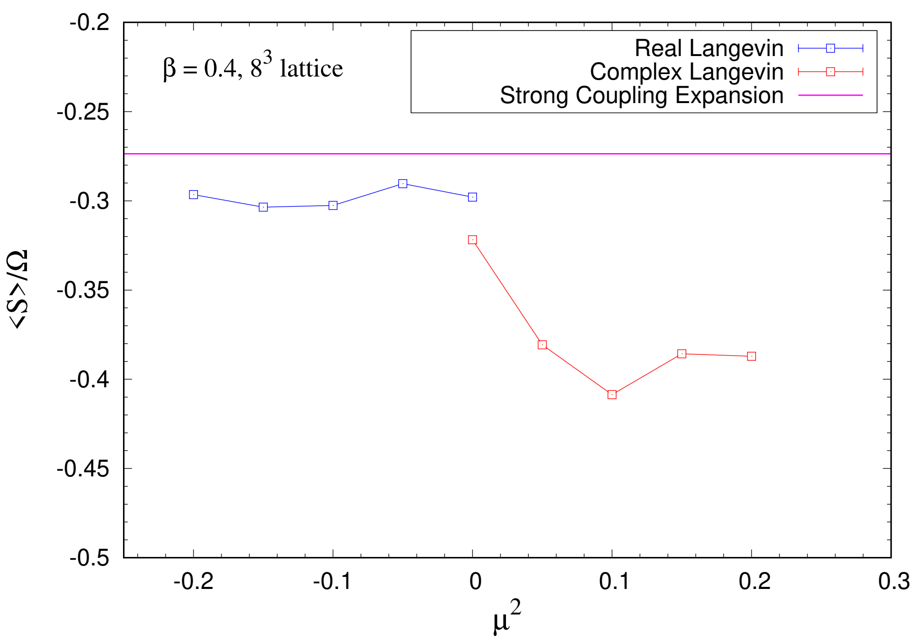
3D XY Model Action Density

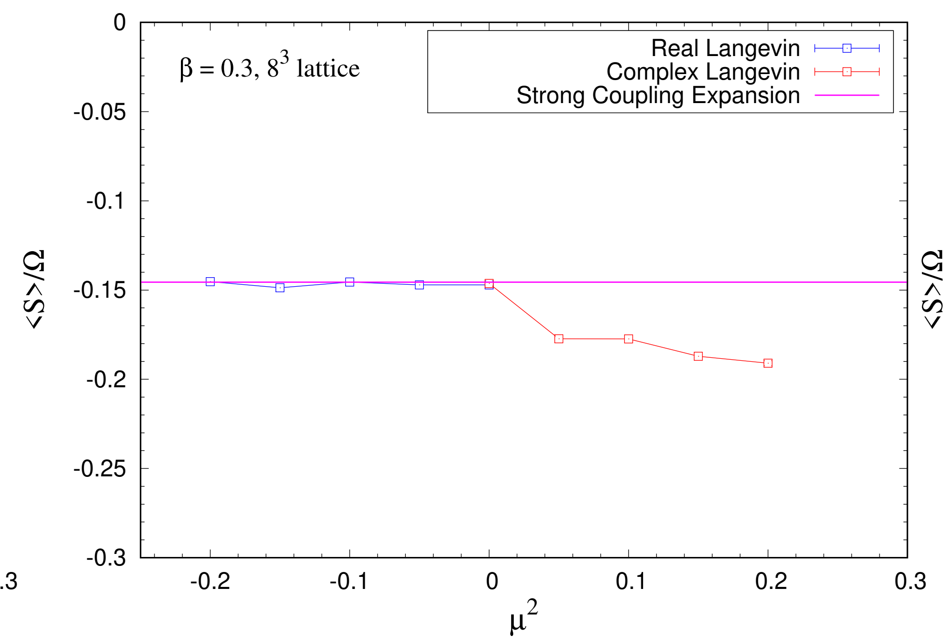
S/Ω ordered phase , $O(2)$ spon. broken $\beta > \beta_c \simeq 0.454$

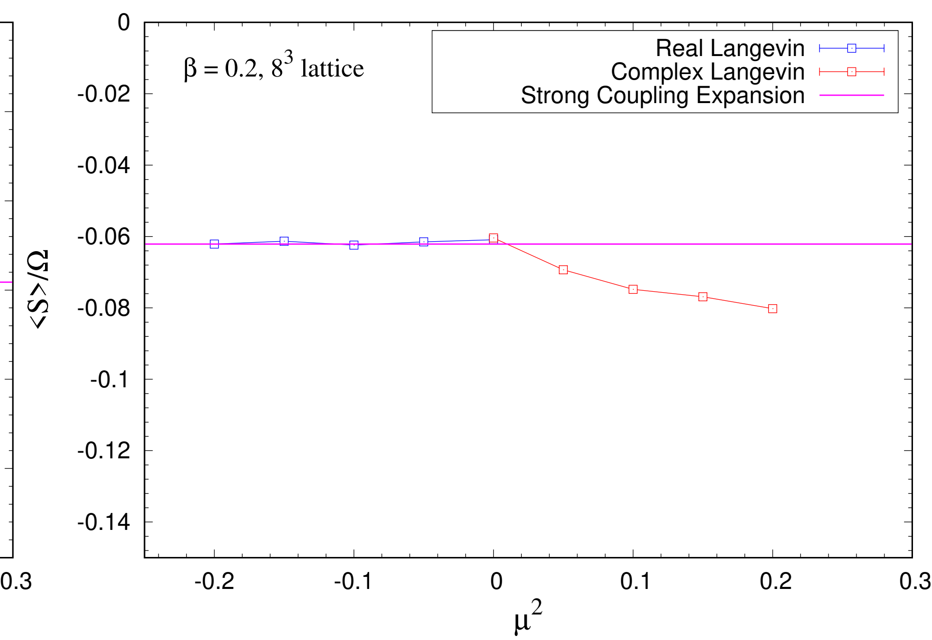


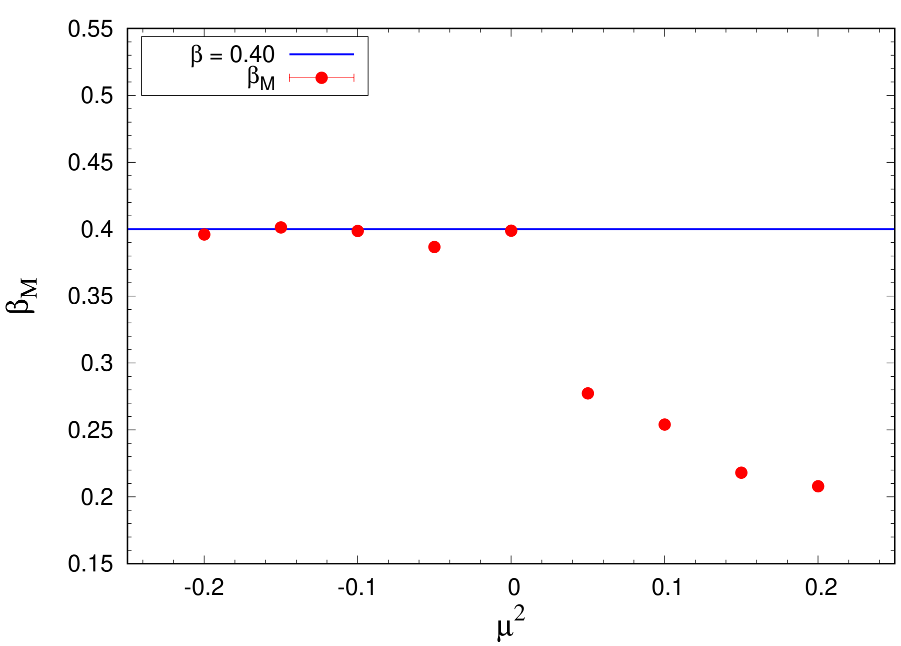
3D XY Model Action Density

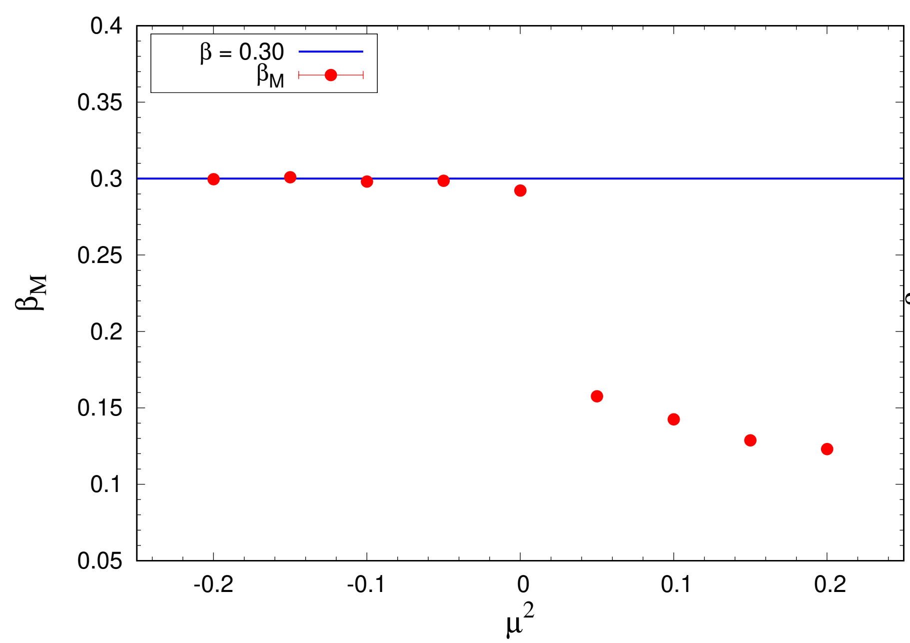
S/Ω disordered phase, $O(2)$ sym $\beta < \beta_c \simeq 0.454$

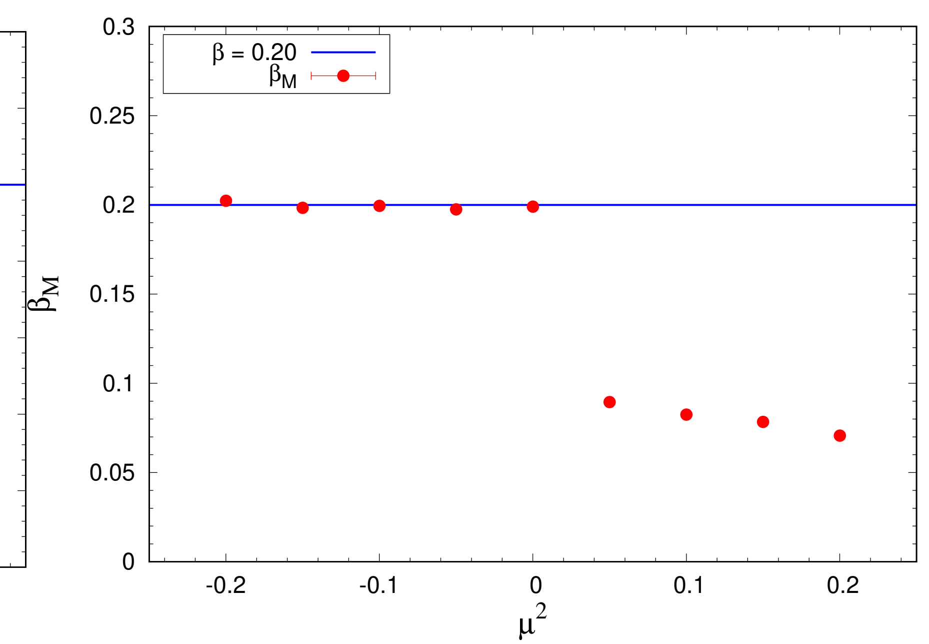












Brief Outlook for Configuration-based Thermometer

Diagnostic toolkit and Reliability Criterion for CLM

Strengthens link between numerical correctness and physical consistency.

Broad spectrum of applications:

- Lattice QCD at finite density
- Quantum mechanical matrix models and supersymmetric theories
- Sensitive indicator of phase transitions in complex-action systems!

Future directions:

- Lattice gauge theories; directly linked to the bare coupling
- Discretization artefacts: validation for continuum extrapolations

Thank you for attention!

Questions, Comments, Suggestions!