Configurational Temperature as a Diagnostic Tool for the 3D XY Model

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Outline

QCD Phase Diagram

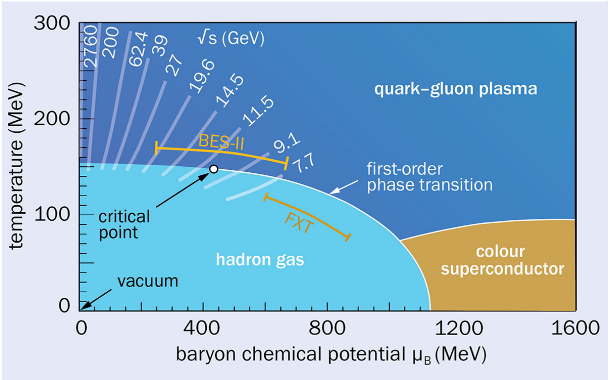


Figure: Conjectured QCD phase diagram

Possible to develop insight by studying the 3D XY Model

The 3D XY Model

- Hamiltonian of the 2+1-dimensional XY Model($\vec{S} = (\cos(\phi), \sin(\phi))$)

$$H = -J \sum_{i \neq j} \vec{S}_i \cdot \vec{S}_j = -J \sum_{x} \sum_{\nu=0}^{2} \cos(\phi_x - \phi_{x+\hat{\nu}})$$

- Euclidean action:

$$S_E = \frac{H}{k_B T} = -\frac{J}{k_B T} \sum_{x} \sum_{\nu=0}^{2} \cos(\phi_x - \phi_{x+\hat{\nu}})$$

$$\beta = \frac{J}{k_B T}$$

Introducing a Chemical Potential

- A chemical potential can be introduced by modifying the temporal term, leading to the action

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

- Monte Carlo algorithms are based on

$$Z = \int [d\theta_x] e^{-S},$$

- When $\mu \neq 0$ the action becomes complex, they suffer from a sign problem.

Imaginary Chemical Potential

- Purely imaginary $\mu = i\mu_I$ (with μ_I real) makes the action real again:

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

- Enables conventional importance sampling

Configurational Temperature Estimator

- General definition (canonical ensemble):

$$\hat{\beta} = \frac{\langle \nabla^2 S \rangle}{\langle |\vec{\nabla} S|^2 \rangle}$$

- Provides a powerful, independent consistency check for numerical simulations – especially valuable when standard diagnostics fail (e.g., complex Langevin).

Application to the XY Model

- Gradients and Laplacians:

$$\frac{\partial S}{\partial \phi_x} = \beta \sum_{\nu=0}^{2} \Big[\sin(\phi_x - \phi_{x+\hat{\nu}} - i\mu\delta_{\nu,0}) - \sin(\phi_{x-\hat{\nu}} - \phi_x - i\mu\delta_{\nu,0}) \Big]$$

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

- Per-configuration averages:

$$g^2 = \frac{1}{\Omega} \sum_x (\partial_{\phi_x} S)^2, \quad H = \frac{1}{\Omega} \sum_x \partial^2_{\phi_x} S$$

- Estimator: $\hat{\beta} = \dfrac{H}{g^2}$ and $\beta_M = \langle \hat{\beta} \rangle$.

Benchmark for simulations

- Worldline formalism gives:

$$f = -\frac{3}{4}\beta^2 - \frac{21}{64}\beta^4 + \mathcal{O}(\beta^6)$$

- The action density follows from

$$\frac{\langle S\rangle}{\Omega} = \frac{\partial f}{\partial \beta} = -\frac{3}{2}\beta^2 - \frac{21}{16}\beta^4 + O(\beta^6)$$

.

- At $\mu = 0$:

$$\frac{\langle S\rangle}{\Omega} = \begin{cases} -0.0621 + \mathcal{O}(10^{-4}), & \beta = 0.2, \\ -0.1450 + \mathcal{O}(10^{-3}), & \beta = 0.3. \end{cases} \tag{1}$$

Action Density – Comparison with Strong-Coupling Expansion

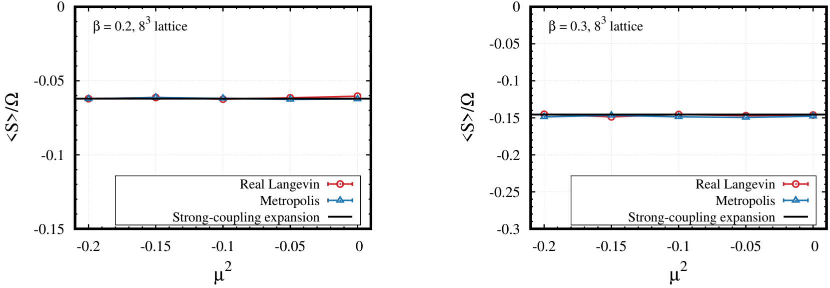
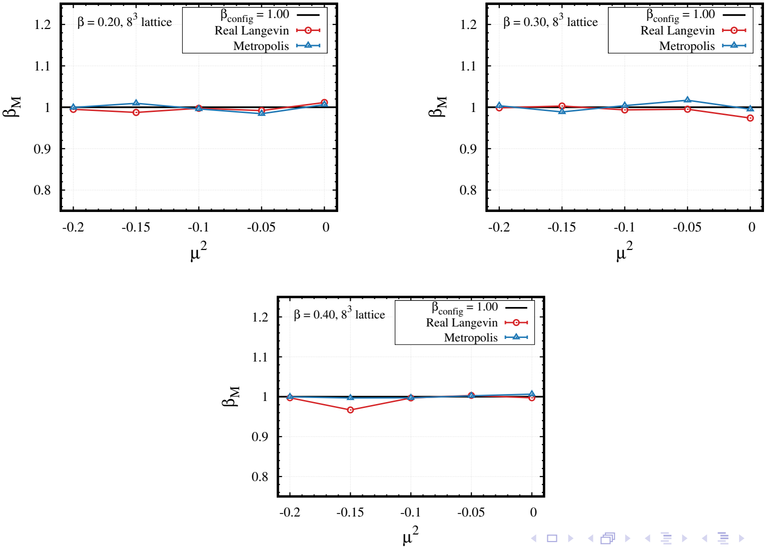


Figure: The action density $\langle S \rangle / \Omega$ as a function of μ^2 on an 8^3 lattice

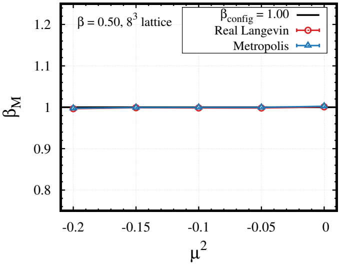
Excellent agreement in the weak-coupling limit($\beta \ll 1$)

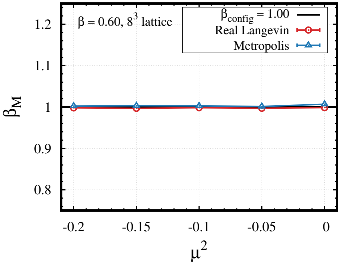
Weak coupling ($\beta = 0.2, 0.3, 0.4$)

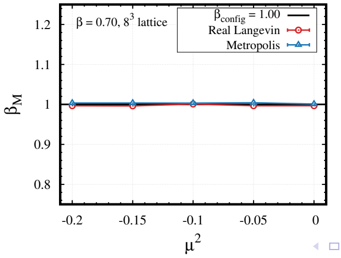


Configurational Temperature β_M vs μ^2

Strong coupling ($\beta = 0.5, 0.6, 0.7$)







Systematic Effects

- **Finite-size effects**
- **Discretisation artifacts**
- **Autocorrelations**

Conclusions and Further Work

- The results give validity to the diagnostic tool
- Perform finite-size scaling to remove volume effects
- Implement in finer lattices
- Extend to real μ (complex Langevin) and use β_M to detect wrong convergence.
- Apply the same diagnostic to other lattice field theories (e.g., scalar QED, QCD at finite density).

References I

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Thank you!

Questions?

Roberge–Weiss Periodicity and Final-Time-Slice Formulation

- Naive discretisation can miss the RW transition.
- **Final-time-slice (fts) formulation**: field redefinition $\phi_{x,\tau} \to \phi'_{x,\tau} = \phi_{x,\tau} - \mu_I \tau$(Shift the temporal phases)
- $\cos(\phi_{x,\tau} - \phi_{x,\tau+1} + \mu_I)$

$$S_{\text{fts}} = -\beta \sum_{x,\nu} \cos\big(\phi_x - \phi_{x+\hat{\nu}} - i N_\tau \mu \, \delta_{\tau,N_\tau} \delta_{\nu,0}\big)$$

- Valid for arbitrary complex μ; correctly reproduces RW transitions even at strong coupling.