

Configurational Temperature in Matrix Models, Metastable states in $2 + 1$ flavor QCD

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Configurational Temperature Estimator in Matrix Models

Anosh Joseph, VM

[arXiv:2606.28148\[hep-th\]](https://arxiv.org/abs/2606.28148)

Outline

- Motivation
- Configurational Temperature from Schwinger-Dyson Identity
- Matrix Model Results
- Use as Monte Carlo Diagnostic

Motivation

- In canonical Monte Carlo simulations, is there a non-kinetic way to directly calculate temperature from field configurations?
- For microcanonical ensembles, an approach for measuring temperature based on a geometric analysis of phase space was developed by Rugh*.
- Later, it was extended to canonical ensembles by Butler et.al.** .
- However, it's applicability in field theory and relationship with Schwinger-Dyson identity, has only recently been explored.
- We explore how this estimator approaches expected value in finite N Matrix models .

*H. H. Rugh, “Dynamical Approach to Temperature ”, *Phys. Rev. Lett.* 78. 772 (1997)

* * Butler et.al., “Configurational Temperature”, *J. Chem. Phys.* 109. 6519-6552 (1998)

- Thermodynamic relation: $dE = TdS - PdV$, $\rightarrow \frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_V$
- Consider a micro canonical ensemble with Hamiltonian $H(\vec{\Gamma}(q_1, \dots, q_n, p_1, \dots, p_n))$, where $\vec{\Gamma}$ is a point in phase space.
- Now consider, $\vec{q}' = \vec{q} + \Delta E \cdot \vec{n}(\vec{\Gamma})$ with $\vec{n}(\vec{\Gamma})$ is perpendicular direction to constant energy shell in phase space, of energy E.
- $H(\vec{q}') = H(\vec{q}) + \nabla_{\vec{q}} H \cdot (\vec{q}' - \vec{q}) + O((\vec{q}' - \vec{q})^2)$
- For the choice of $\vec{n}(\vec{\Gamma}) = \frac{\nabla_{\vec{q}} H}{\nabla_{\vec{q}} H \cdot \nabla_{\vec{q}} H}$, energy of the new configuration would be given by: $H(\vec{q}') = H(\vec{q}) + \Delta E + O((\Delta E)^2)$.

- When energy is changed by ΔE as per this transformation, what is the change in entropy?

- Entropy corresponding to the shift of $\vec{n}(\vec{\Gamma})$ can be written as

$$S(E + \Delta E) = k_B \ln(\Omega_{\Gamma'}(E', V, N)) = k_B \ln \int_{\mu_C(E+\Delta E)} d\Gamma' = k_B \ln \int_{\mu_C(E)} \left| \frac{\partial \vec{\Gamma}'}{\partial \vec{\Gamma}} \right| d\Gamma$$

- Now using $\vec{\Gamma}' = \vec{\Gamma} + \Delta E \vec{n}(\vec{\Gamma})$, Jacobian can be written as $1 + \Delta E \vec{\nabla}_{\vec{q}} \cdot \vec{n}(\vec{\Gamma})$.

- $$\Delta S = S(E + \Delta E) - S(E) = k_B \ln \frac{\int_{\mu_C(E)} (1 + \Delta E \vec{\nabla}_{\vec{q}} \cdot \vec{n}(\vec{\Gamma})) d\Gamma}{\int_{\mu_C(E)} d\Gamma} .$$

- Using approximation $\ln(1 + \delta) \approx \delta$, we get $\Delta S = \langle k_B \Delta E \vec{\nabla}_{\vec{q}} \cdot \vec{n}(\vec{\Gamma}) \rangle$

- $$\frac{1}{k_B T} = \left(\frac{\partial S}{\partial E} \right)_V = \langle \vec{\nabla}_{\vec{q}} \vec{n}(\vec{\Gamma}) \rangle = \left\langle \vec{\nabla}_{\vec{q}} \cdot \frac{\nabla_{\vec{q}} H}{\nabla_{\vec{q}} H \cdot \nabla_{\vec{q}} H} \right\rangle.$$

- This gives us expression for inverse temperature $\beta = \left\langle \nabla_{\vec{q}} \frac{\nabla_{\vec{q}} H}{\nabla_{\vec{q}} H \cdot \nabla_{\vec{q}} H} \right\rangle$ in terms of gradient of Hamiltonian corresponding to a configuration.

- The expression can be further simplified in terms Gradient and Hessian of the Hamiltonian. $\vec{g} = \nabla_{\vec{q}} H$, $H_{ij} = \nabla_{\vec{q}_i} \nabla_{\vec{q}_j} H$, $|g|^2 = \vec{g} \cdot \vec{g}$

$$\beta_{\text{config}} = \left\langle \frac{\text{Tr } H}{|g|^2} - 2 \frac{g^T H g}{|g|^4} \right\rangle$$

Configurational Temperature from Schwinger-Dyson Identity

- Considering infinitesimal transformation $\phi_i(x) \rightarrow \phi_i(x) + \epsilon F_i[\phi]$, the corresponding measure modifies to $D\phi' = D\phi (1 + \epsilon \vec{\nabla} \cdot \vec{F})$.
- The action becomes $S_E[\phi + \epsilon F] = S_E[\phi] + \epsilon \vec{F} \cdot \nabla S_E + O(\epsilon^2)$.
- $$Z = \int D\phi' e^{-S_E[\phi']} = \int D\phi e^{-S_E[\phi]} \implies 0 = \int D\phi e^{-S_E[\phi]} \left(\vec{\nabla} \cdot \vec{F} - \vec{F} \cdot \nabla S_E \right)$$
- We get the generalised Schwinger-Dyson identity $\langle \vec{\nabla} \cdot \vec{F} \rangle = \langle \vec{F} \cdot \nabla S_E \rangle$
- Choosing $\vec{F} = \frac{\nabla S_E}{\nabla S_E \cdot \nabla S_E} \implies \vec{F} \cdot \nabla S_E = 1$.

$$\beta_{\text{config}} \equiv \left\langle \nabla \cdot \left(\frac{\nabla S_E}{\nabla S_E \cdot \nabla S_E} \right) \right\rangle \implies \beta_{\text{config}} = 1.$$

Gross-Witten-Wadia Model

$$Z[\lambda] = \int_{\text{U}(N)} dU \, e^{-S[U]} = \int_{\text{U}(N)} dU \, \exp \left[\frac{N}{2\lambda} (\text{Tr} U + \text{Tr} U^\dagger) \right] \qquad U = \text{diag} (e^{i\theta_1}, e^{i\theta_2}, \dots, e^{i\theta_N}),$$

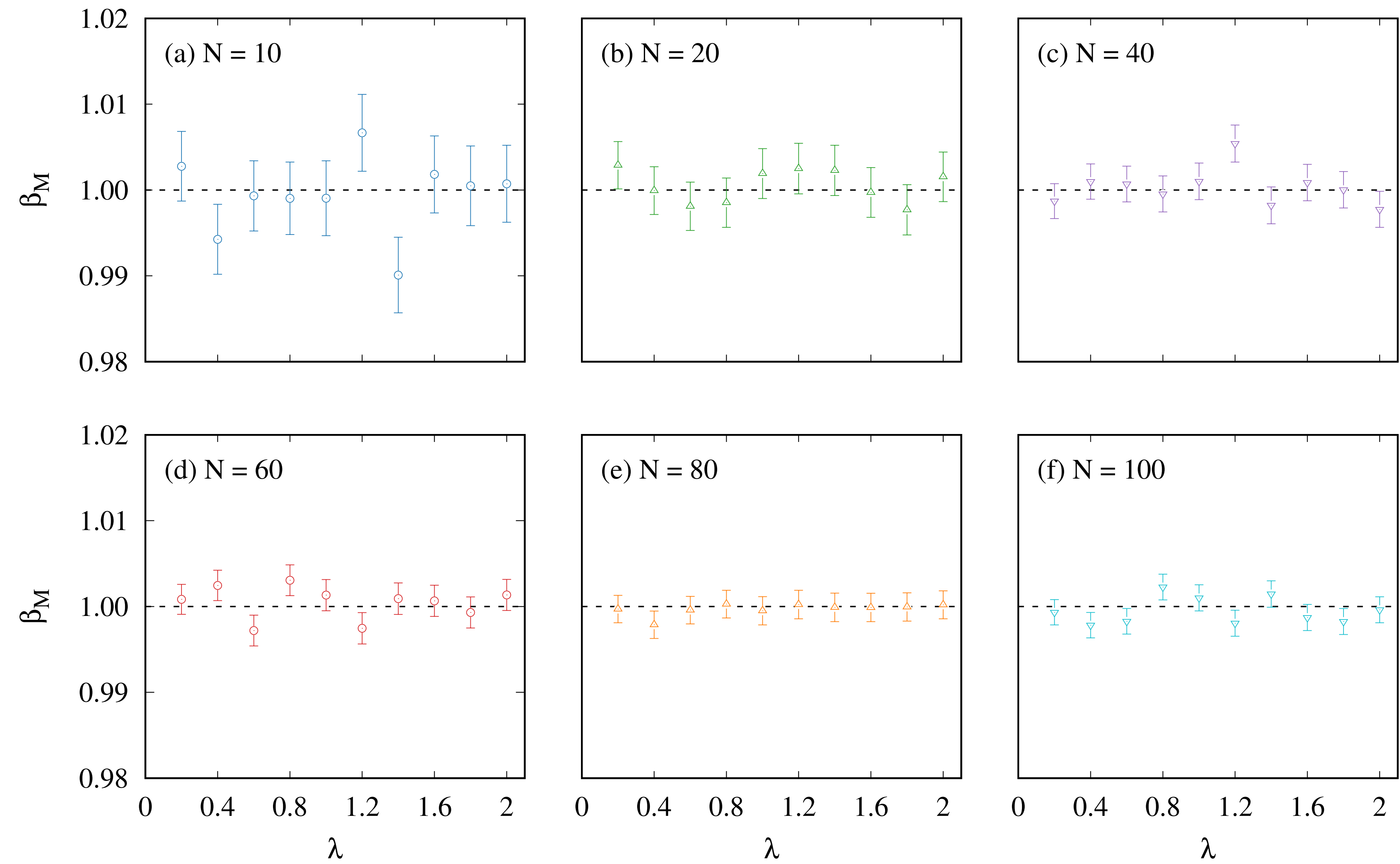
$$S(\theta) = -\frac{N}{\lambda} \sum_{i=1}^N \cos \theta_i - \sum_{i < j} \log \left[\sin^2 \left(\frac{\theta_i - \theta_j}{2} \right) \right].$$

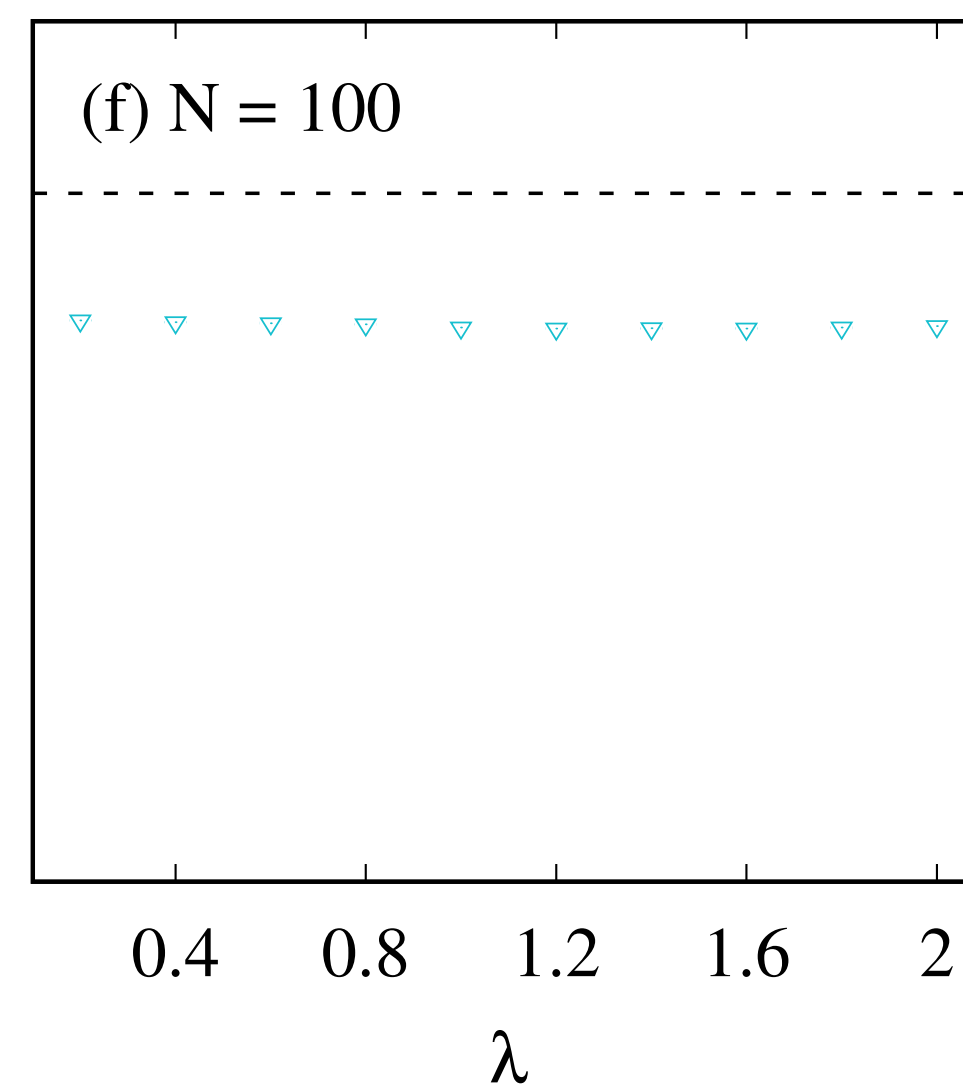
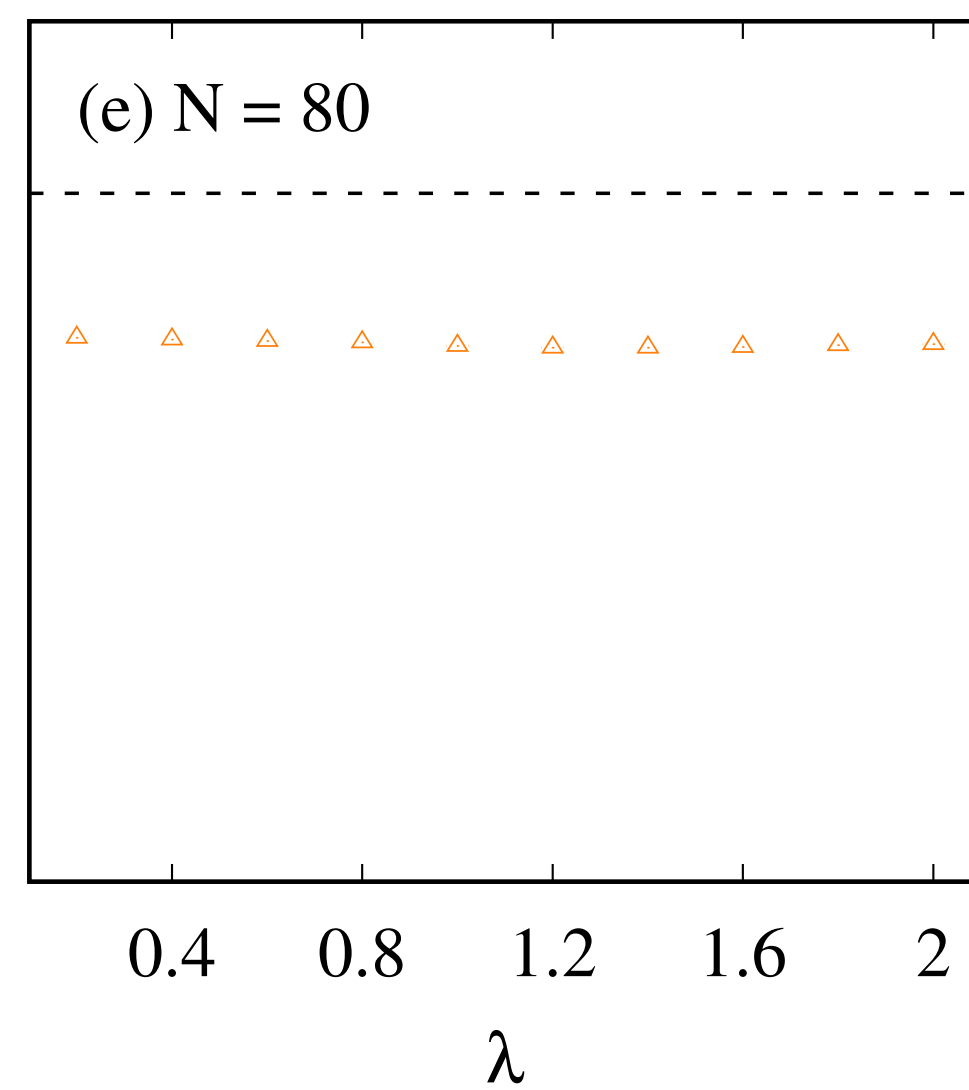
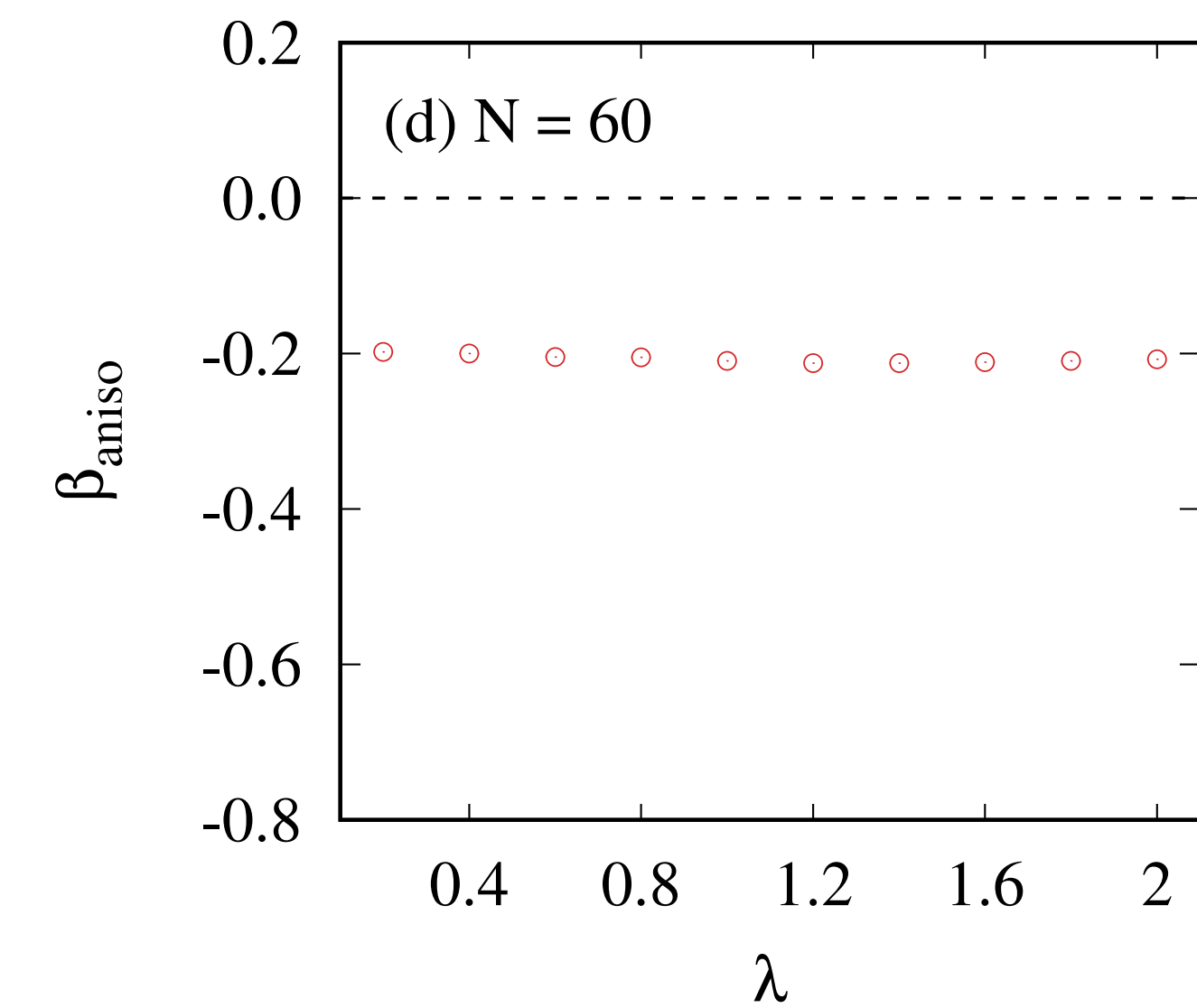
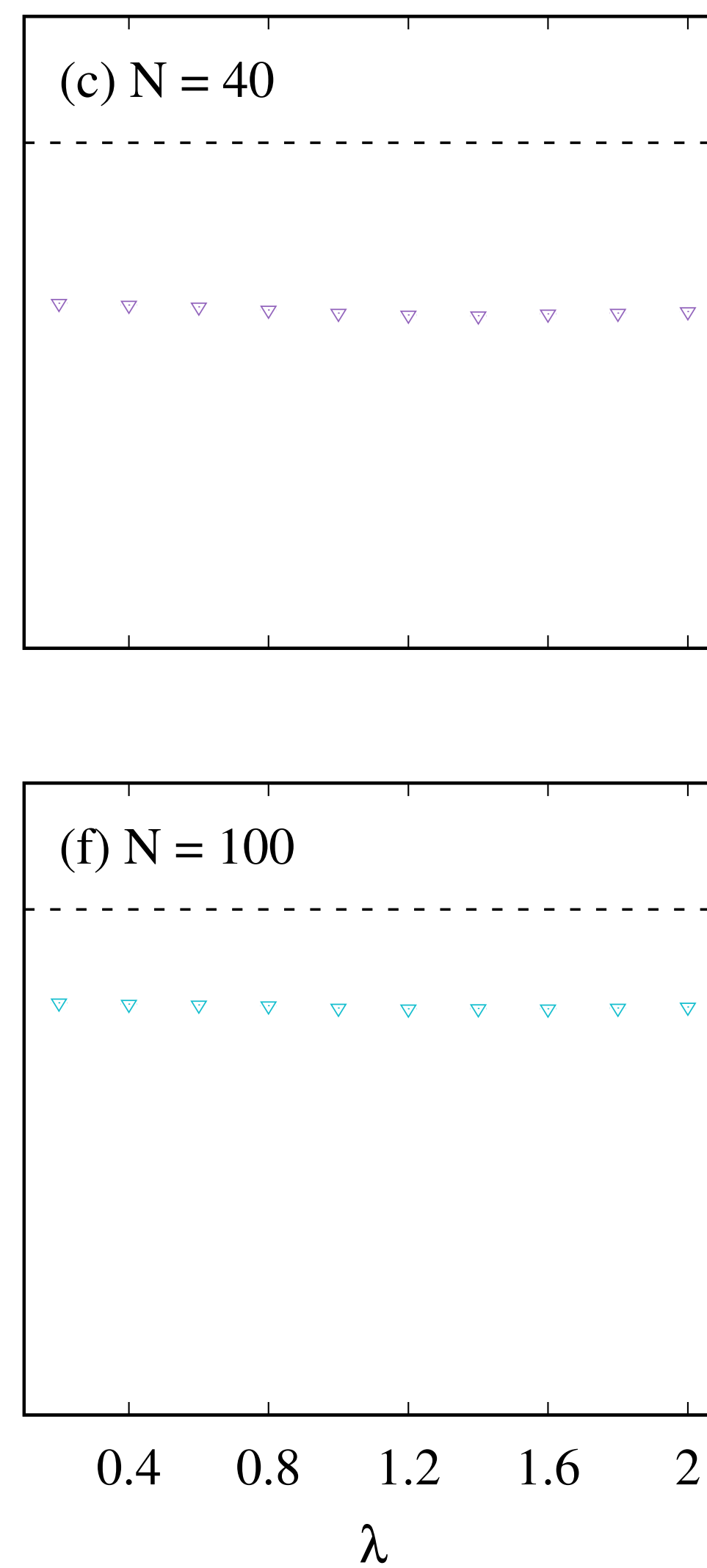
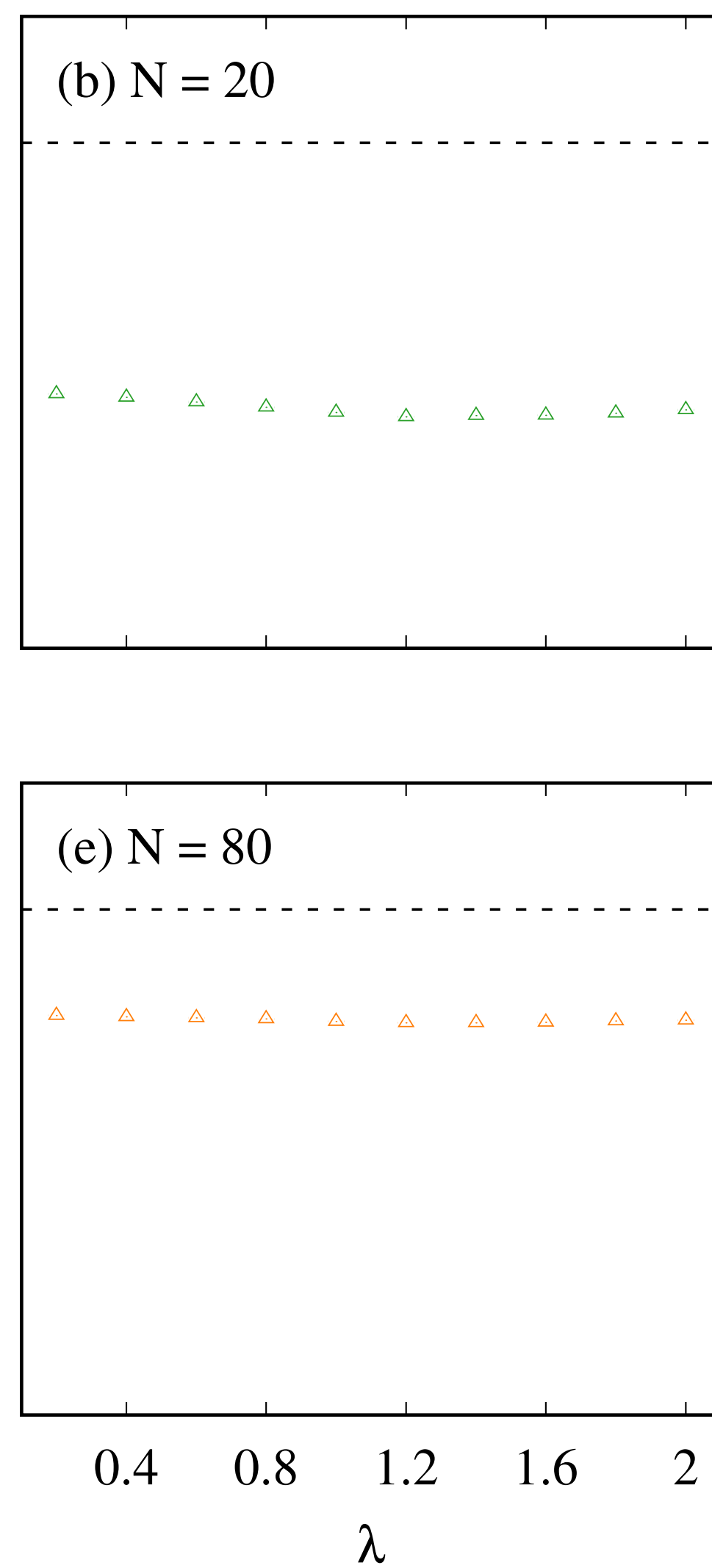
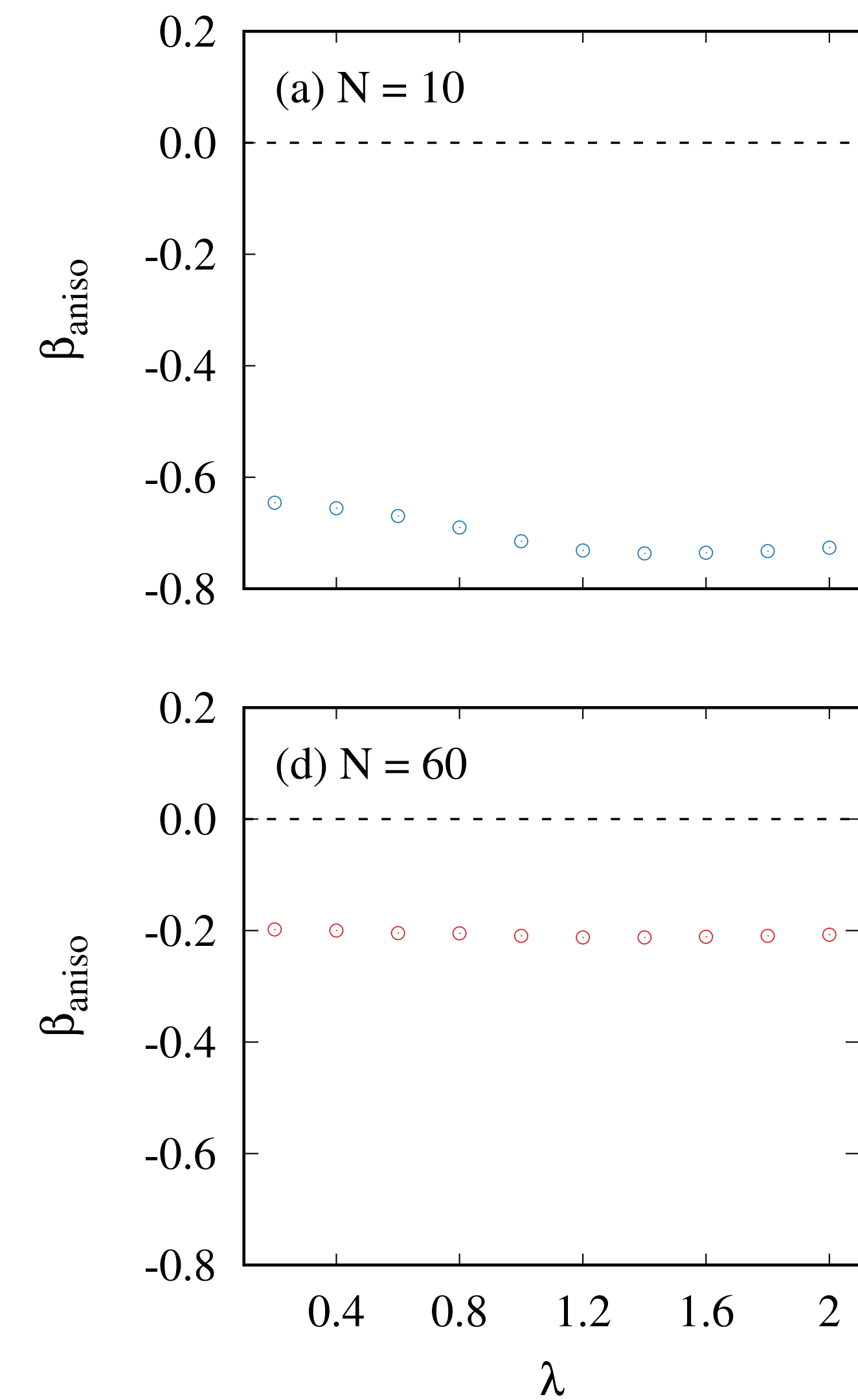
$$g_i = \frac{\partial S}{\partial \theta_i} = \frac{N}{\lambda} \sin \theta_i - \sum_{j \neq i} \cot \left(\frac{\theta_i - \theta_j}{2} \right) \qquad H_{ii} = \frac{N}{\lambda} \cos \theta_i + \frac{1}{2} \sum_{j \neq i} \csc^2 \left(\frac{\theta_i - \theta_j}{2} \right),$$

$$H_{ij} = -\frac{1}{2} \csc^2 \left(\frac{\theta_i - \theta_j}{2} \right), \qquad i \neq j. \qquad \beta_{\text{config}} = \left\langle \frac{\text{Tr} H}{|g|^2} - 2 \frac{g^T H g}{|g|^4} \right\rangle$$

Results

Gross-Witten-Wadia Model



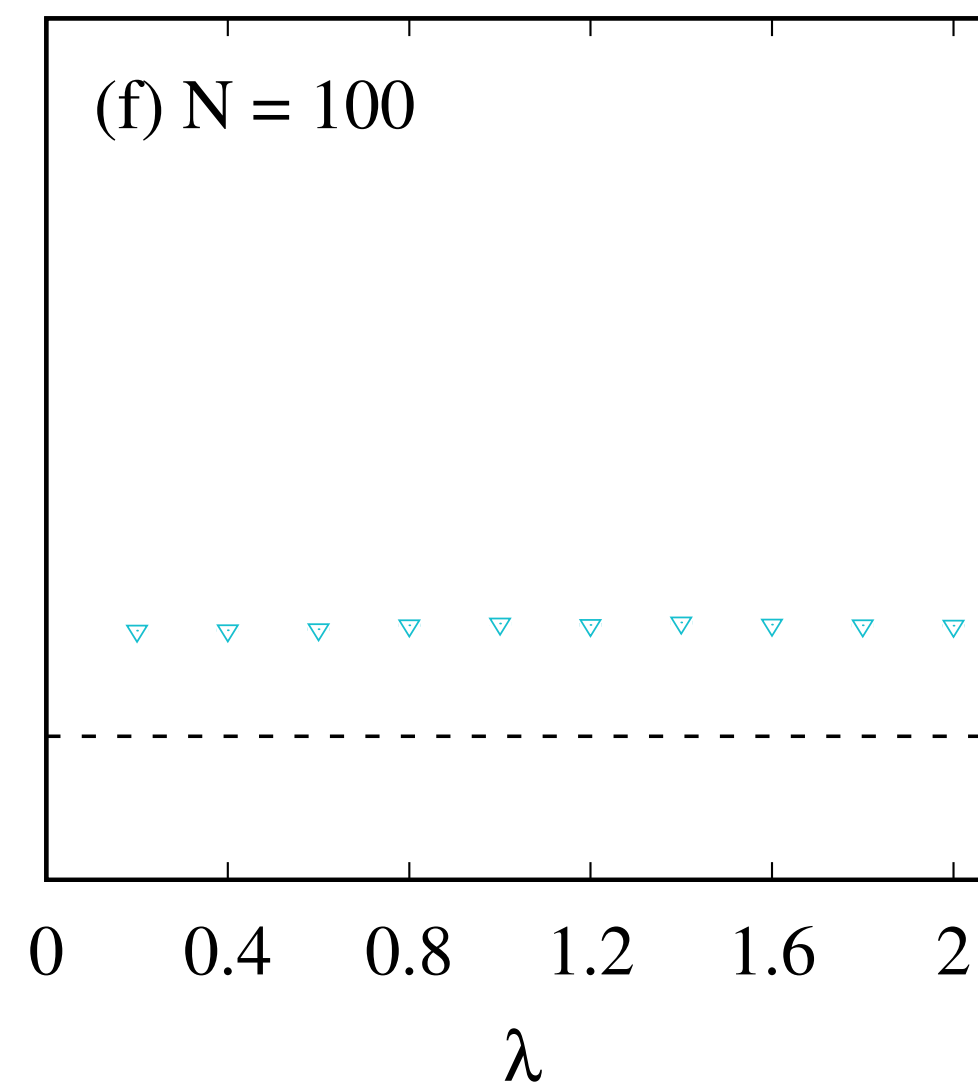
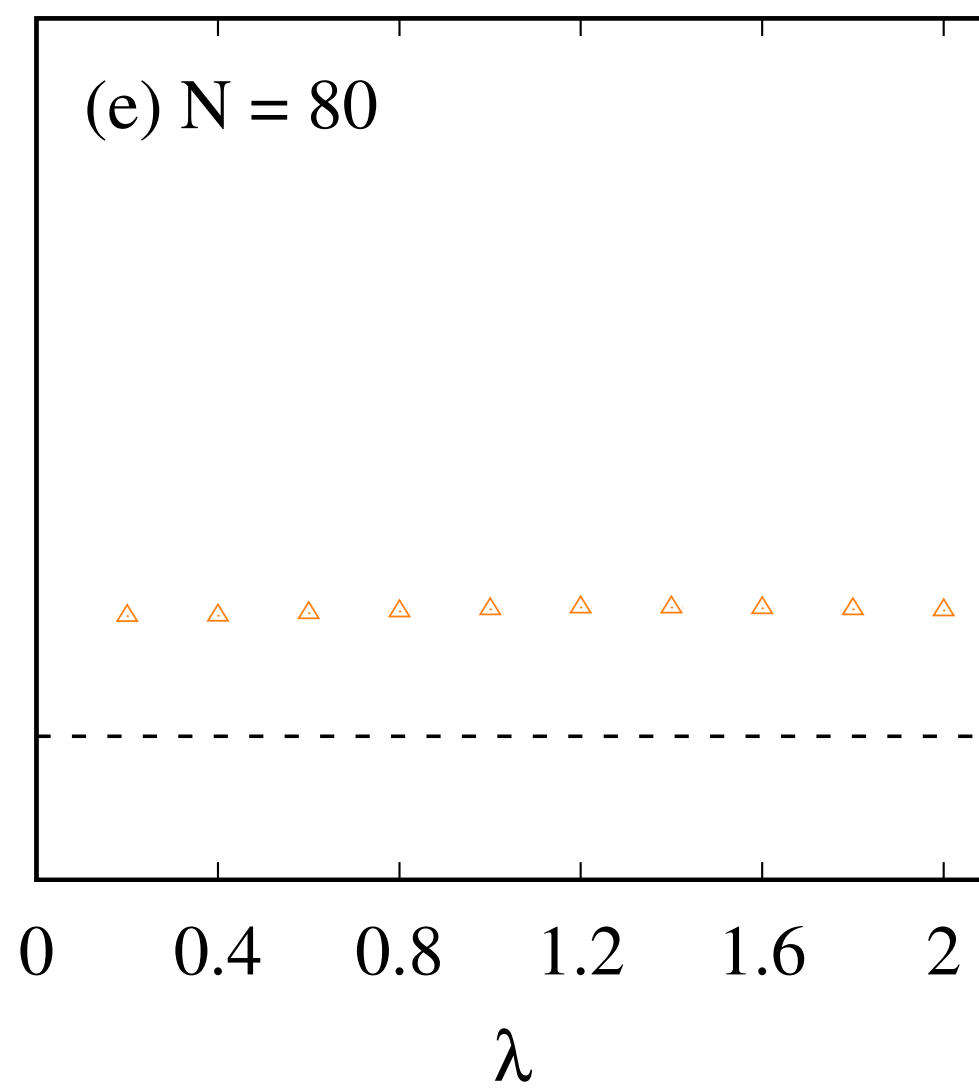
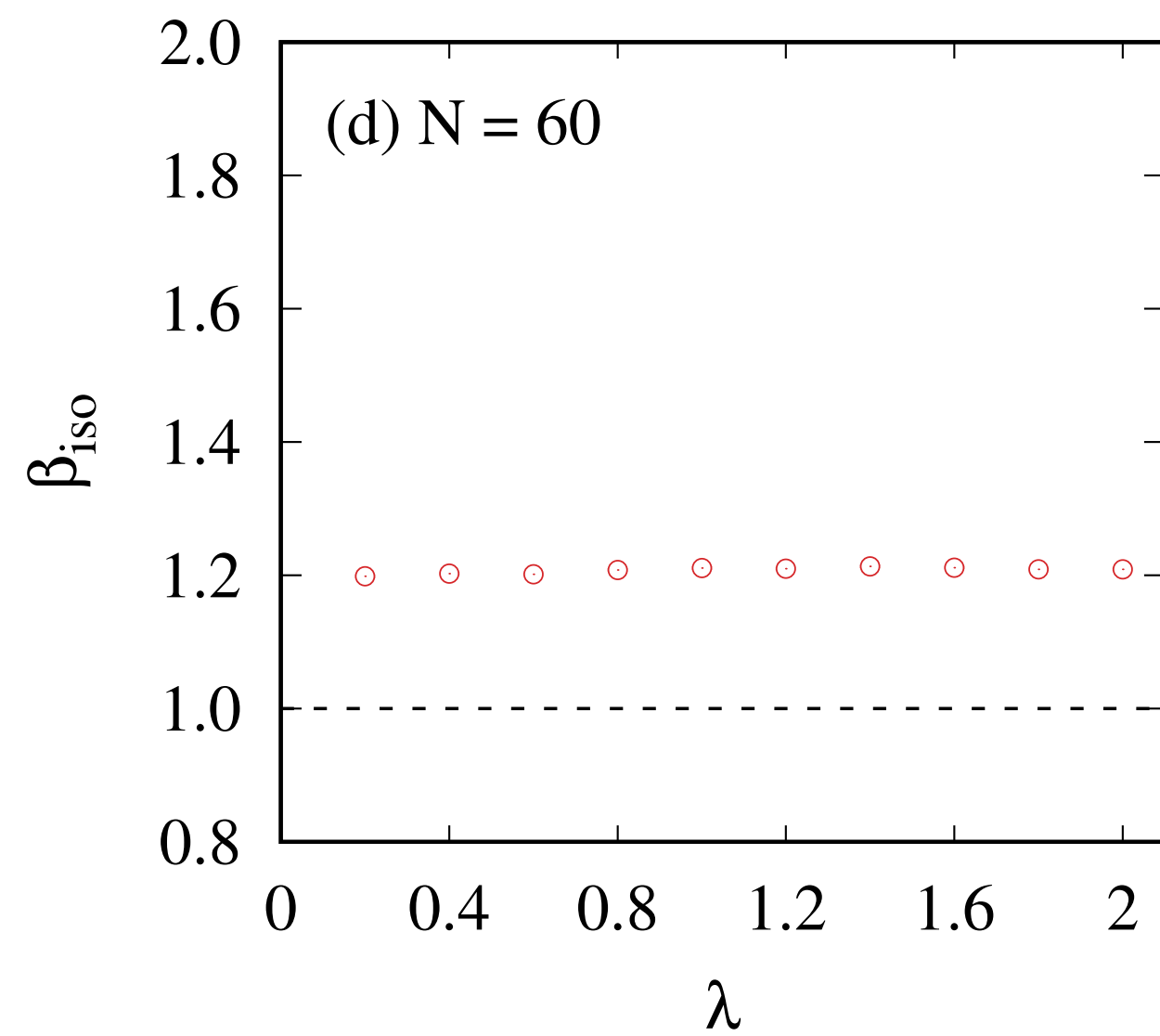
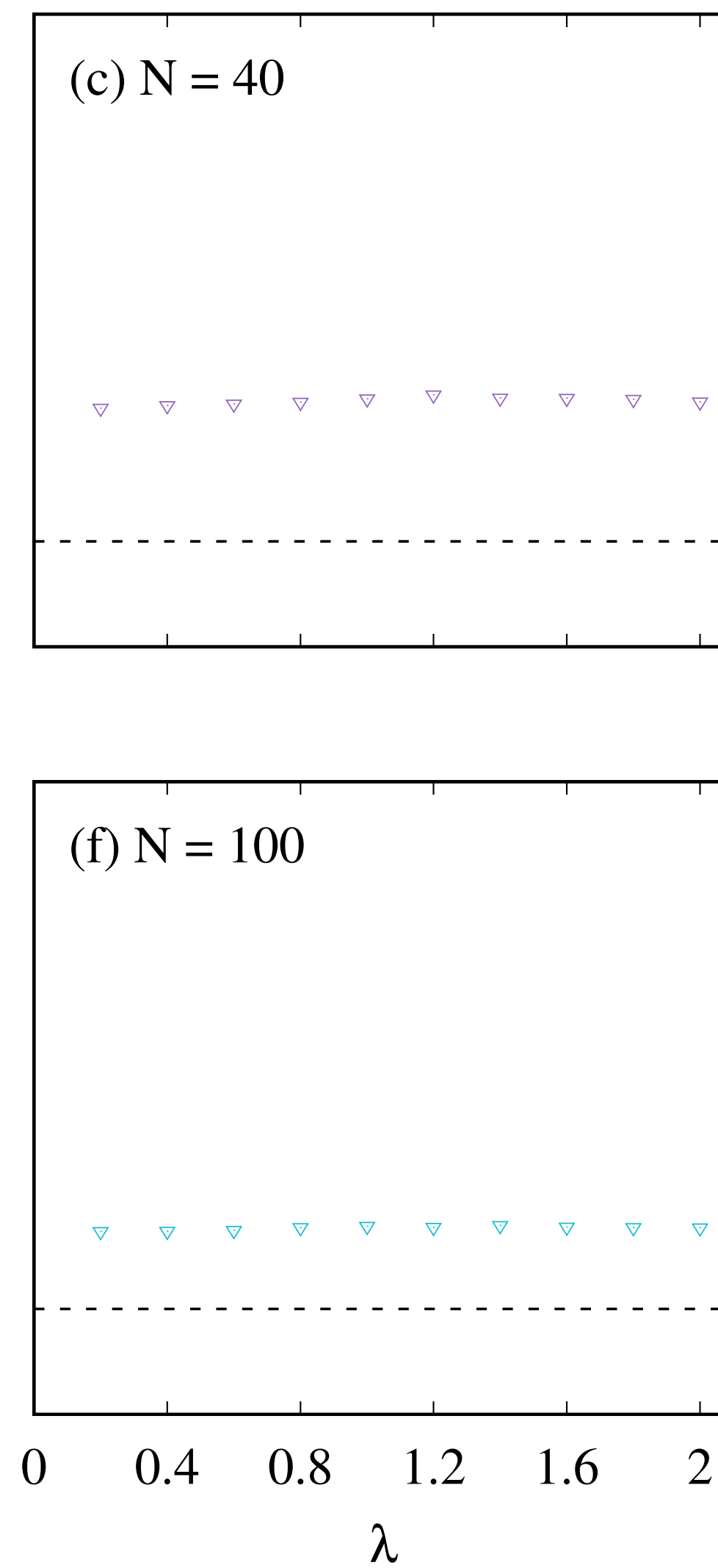
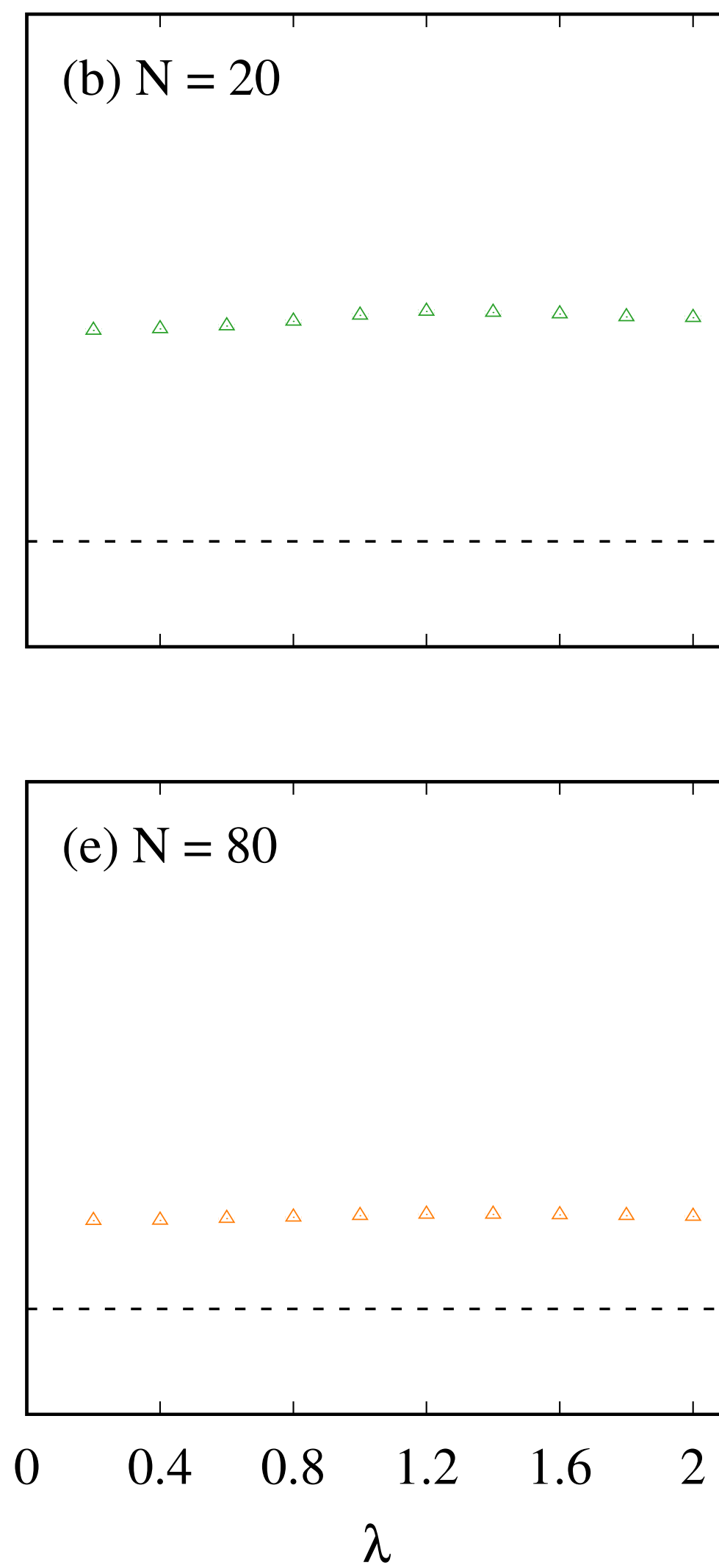
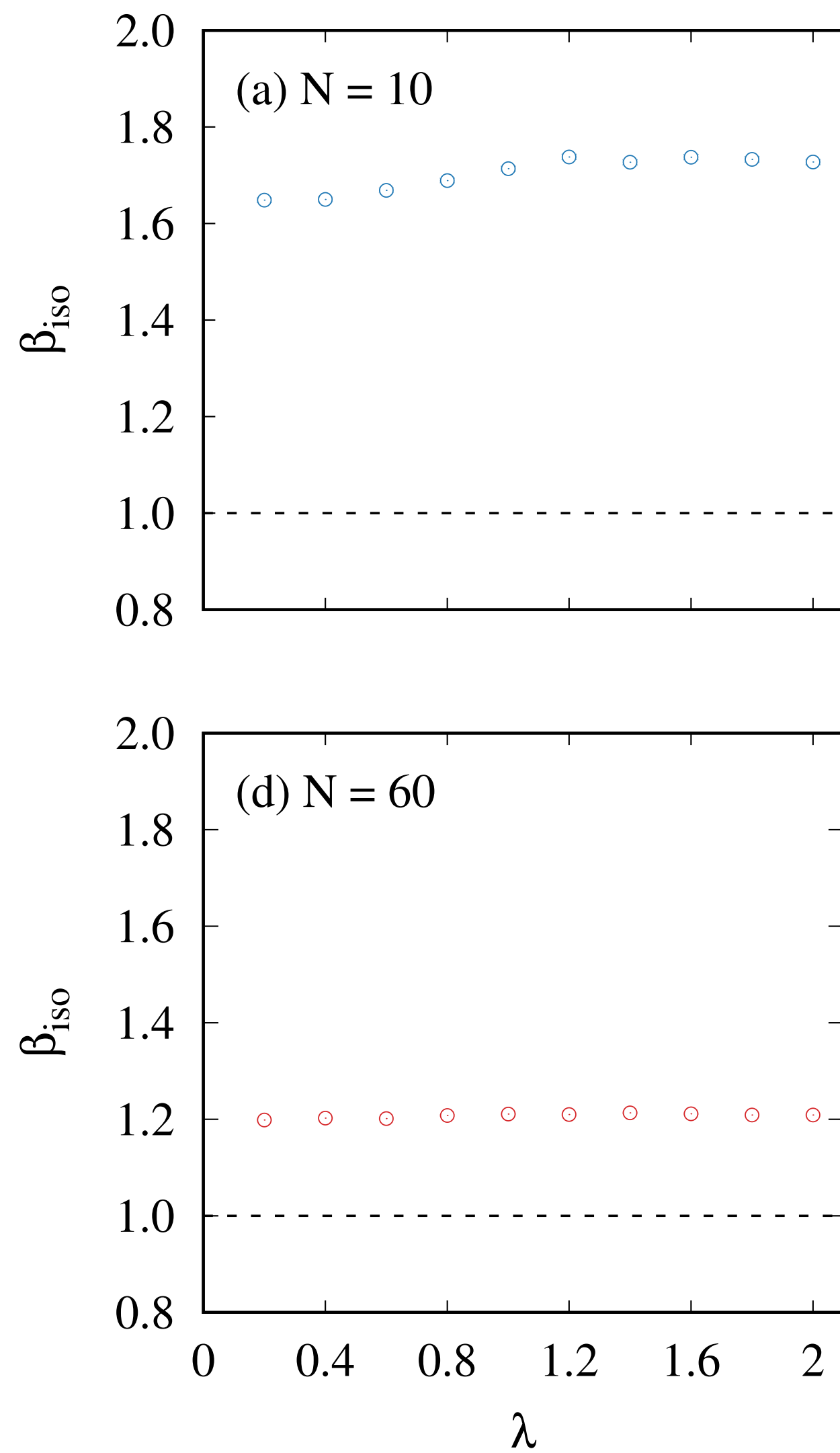


$$\beta_{\text{config}} = \left\langle \frac{\text{Tr } H}{|g|^2} - 2 \frac{g^T H g}{|g|^4} \right\rangle.$$

$$\beta_{\text{config}} = \beta_{\text{iso}} + \beta_{\text{aniso}},$$

$$\beta_{\text{iso}} = \left\langle \frac{\text{Tr } H}{|g|^2} \right\rangle,$$

$$\beta_{\text{aniso}} = -2 \left\langle \frac{g^T H g}{|g|^4} \right\rangle$$



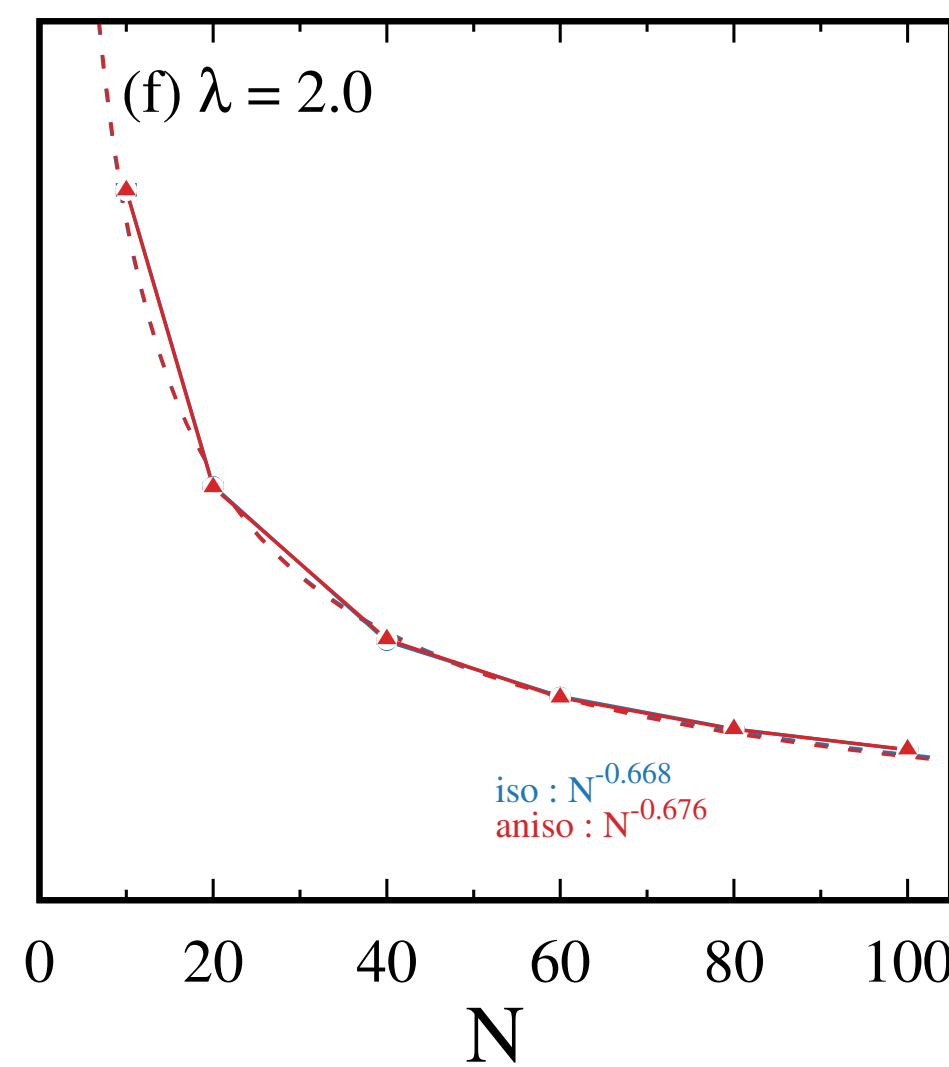
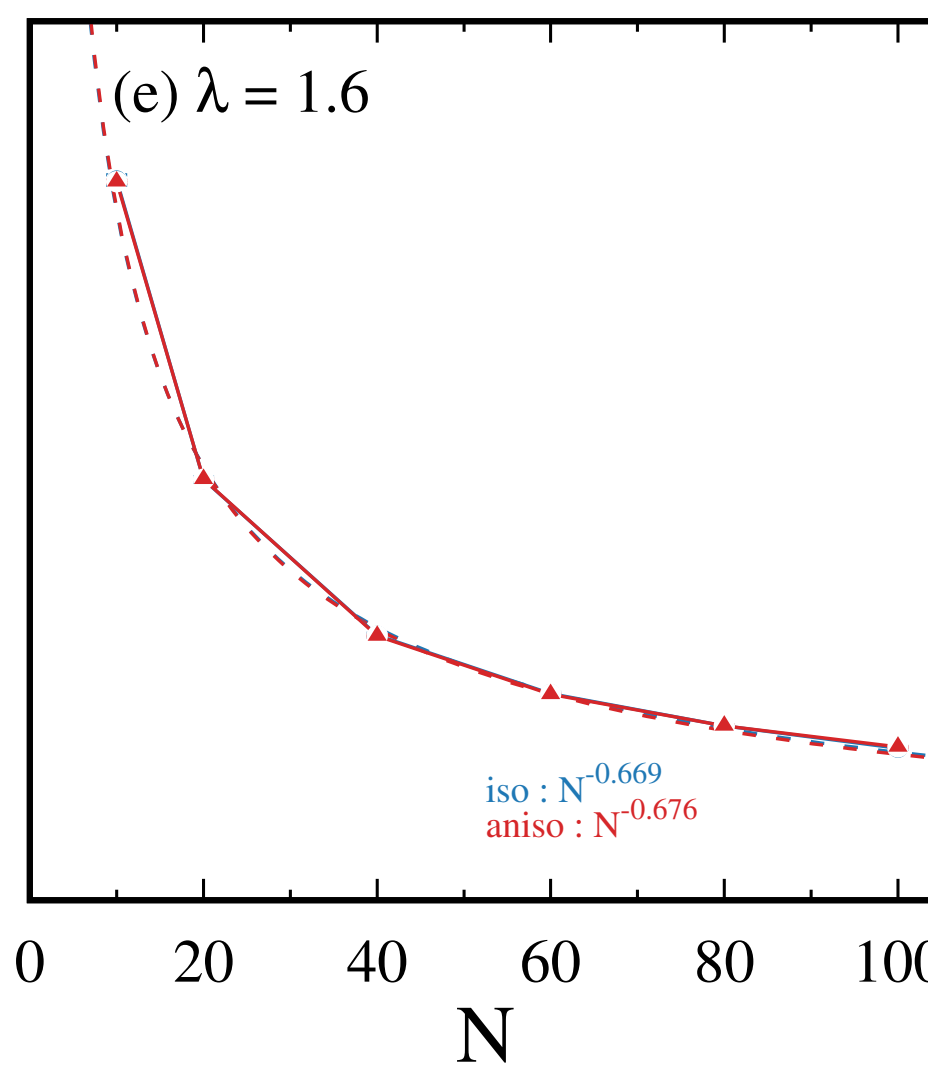
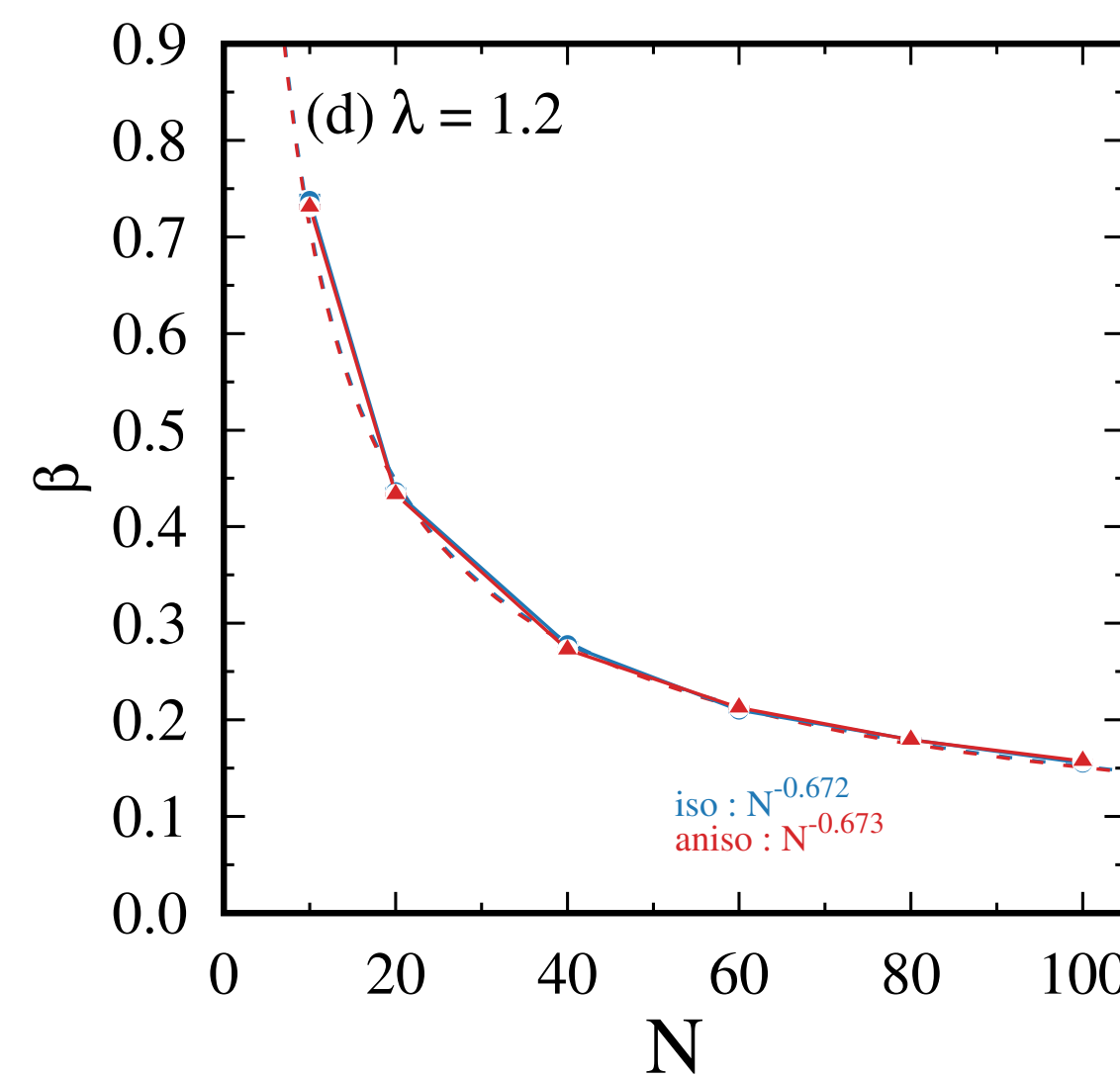
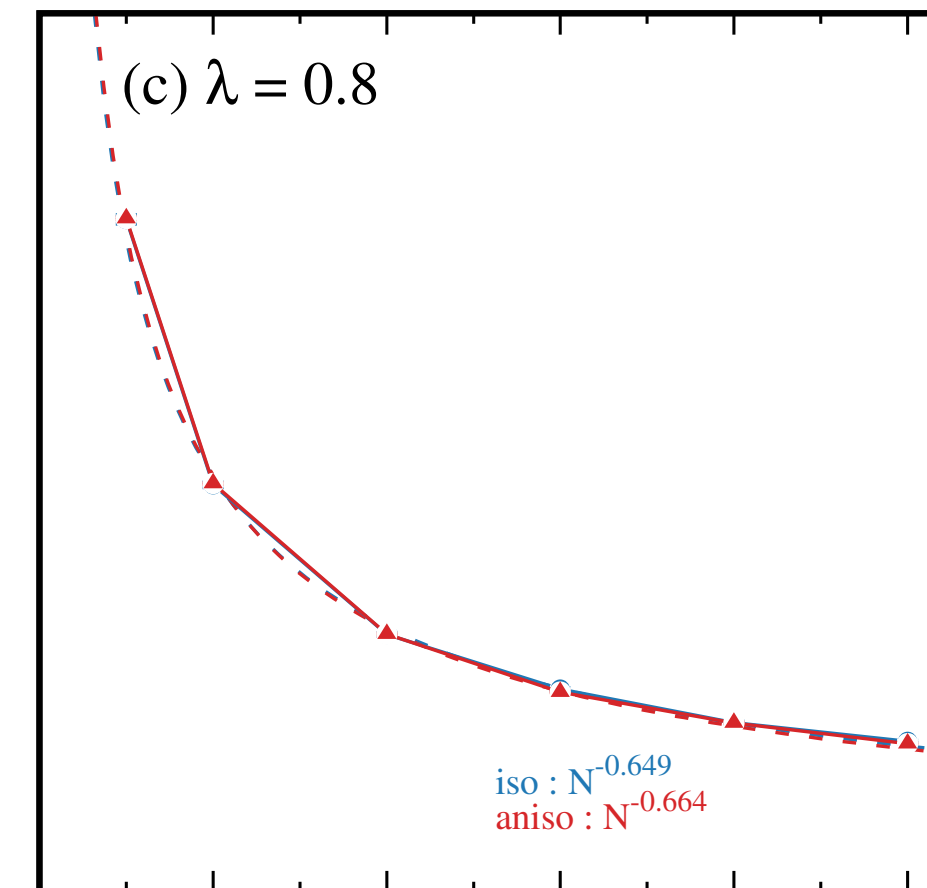
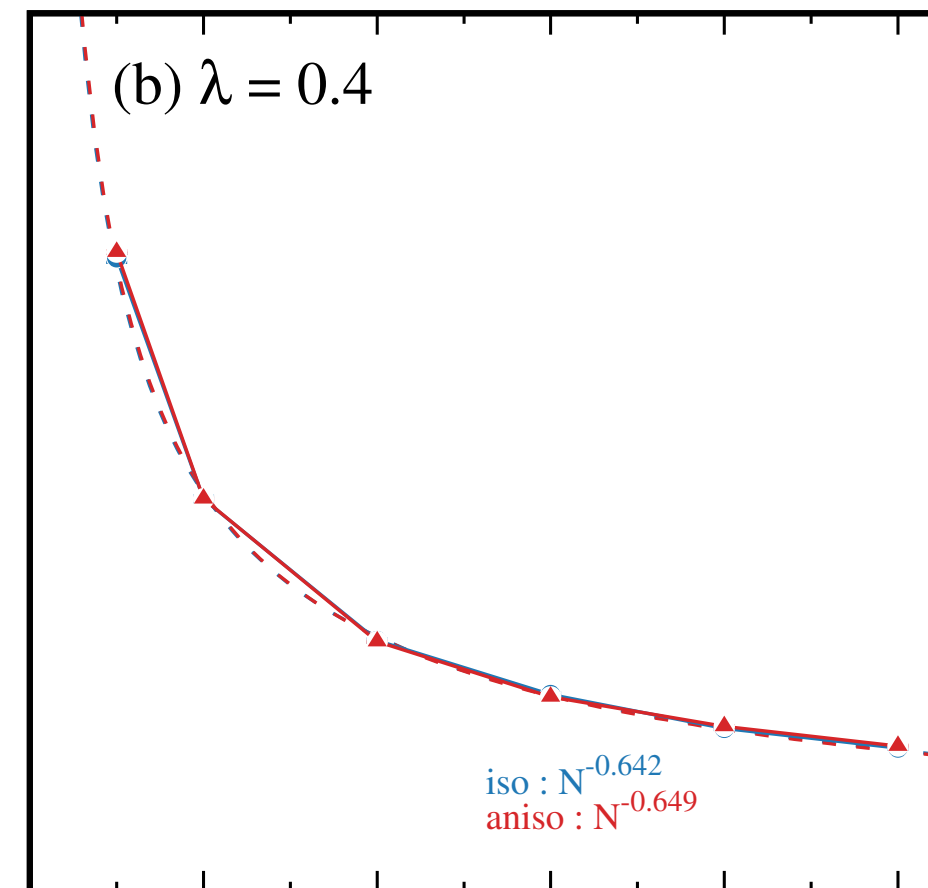
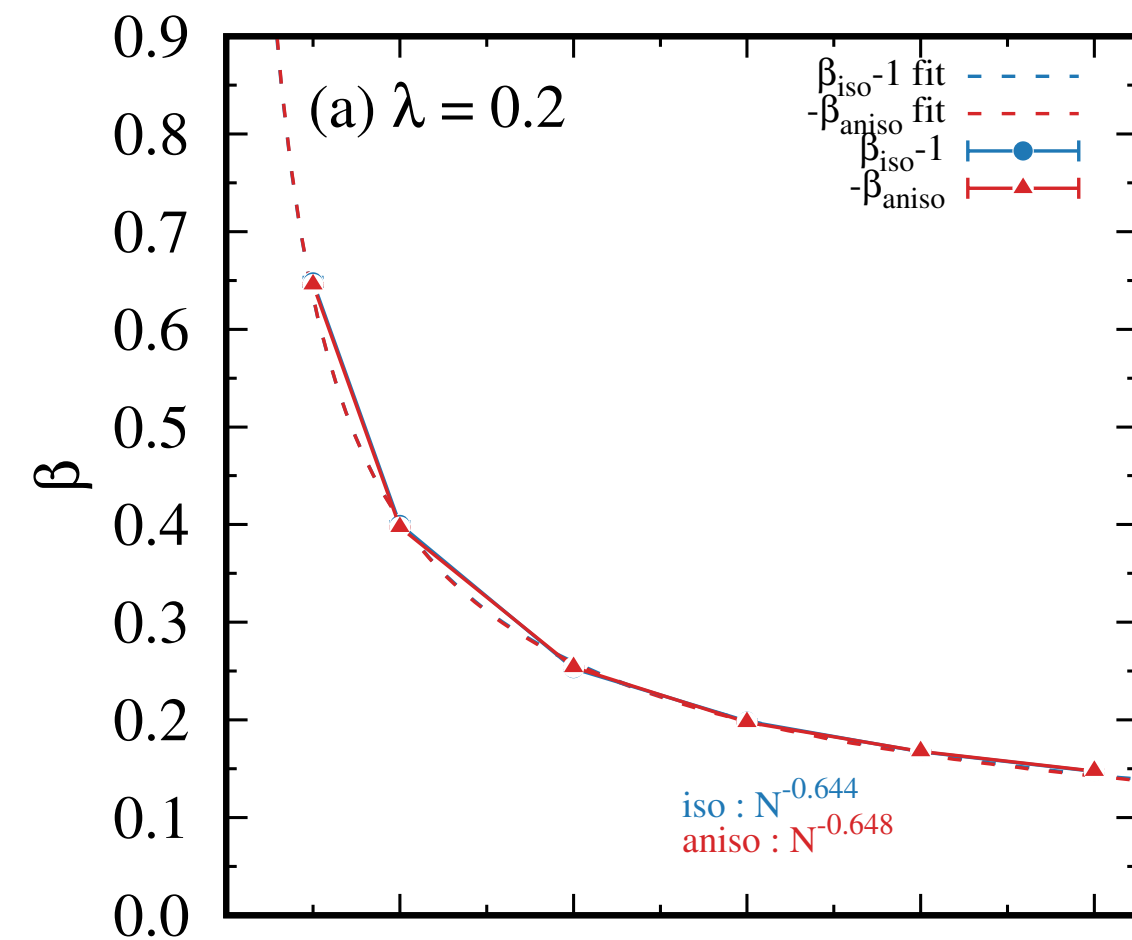
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$$\beta_{\text{iso}} - 1 = A_{\text{iso}} N^{B_{\text{iso}}} \quad -\beta_{\text{aniso}} = A_{\text{aniso}} N^{B_{\text{aniso}}}$$



$$\beta_{\text{config}} = \left\langle \frac{\text{Tr } H}{|g|^2} - 2 \frac{g^T H g}{|g|^4} \right\rangle.$$

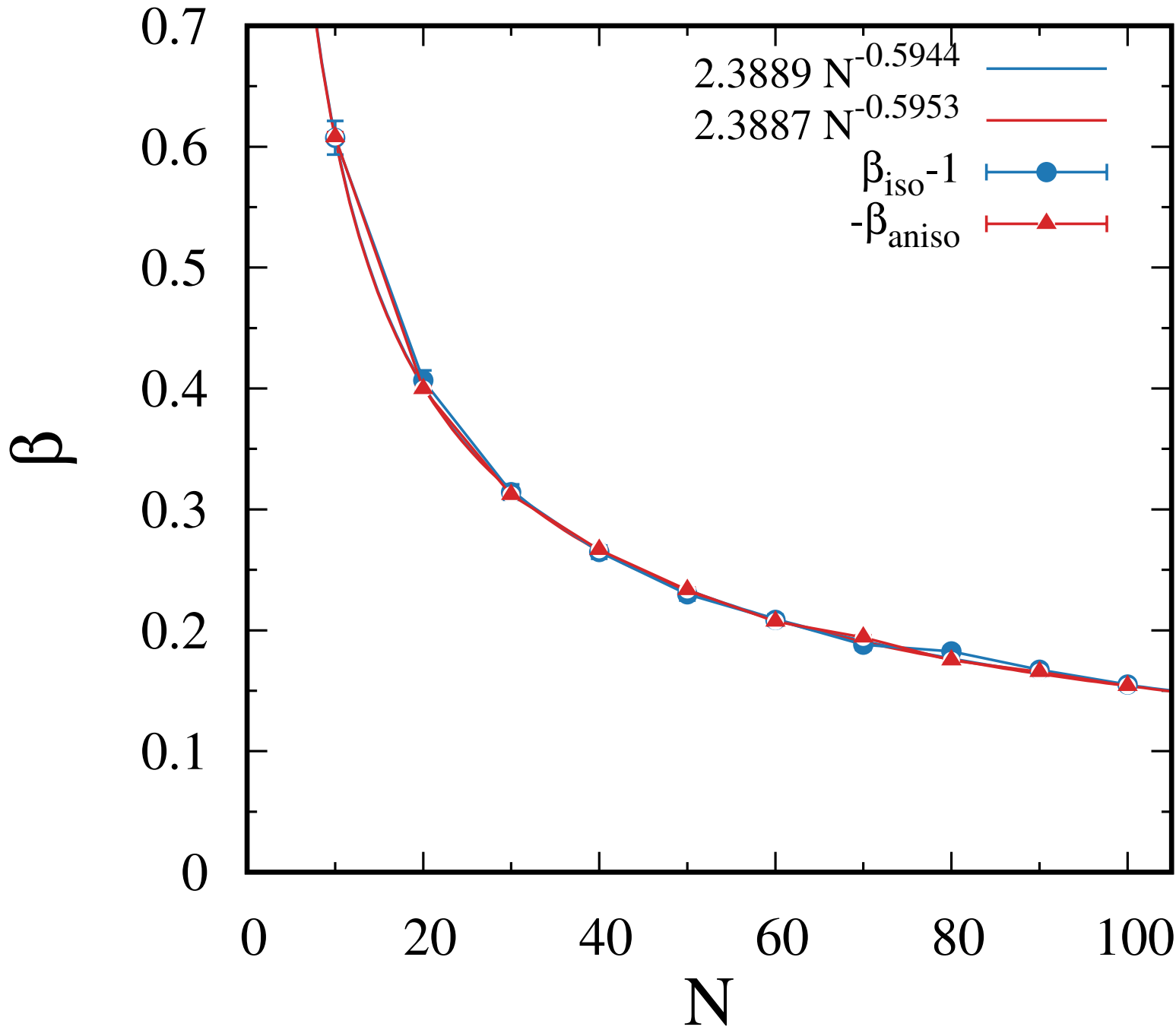
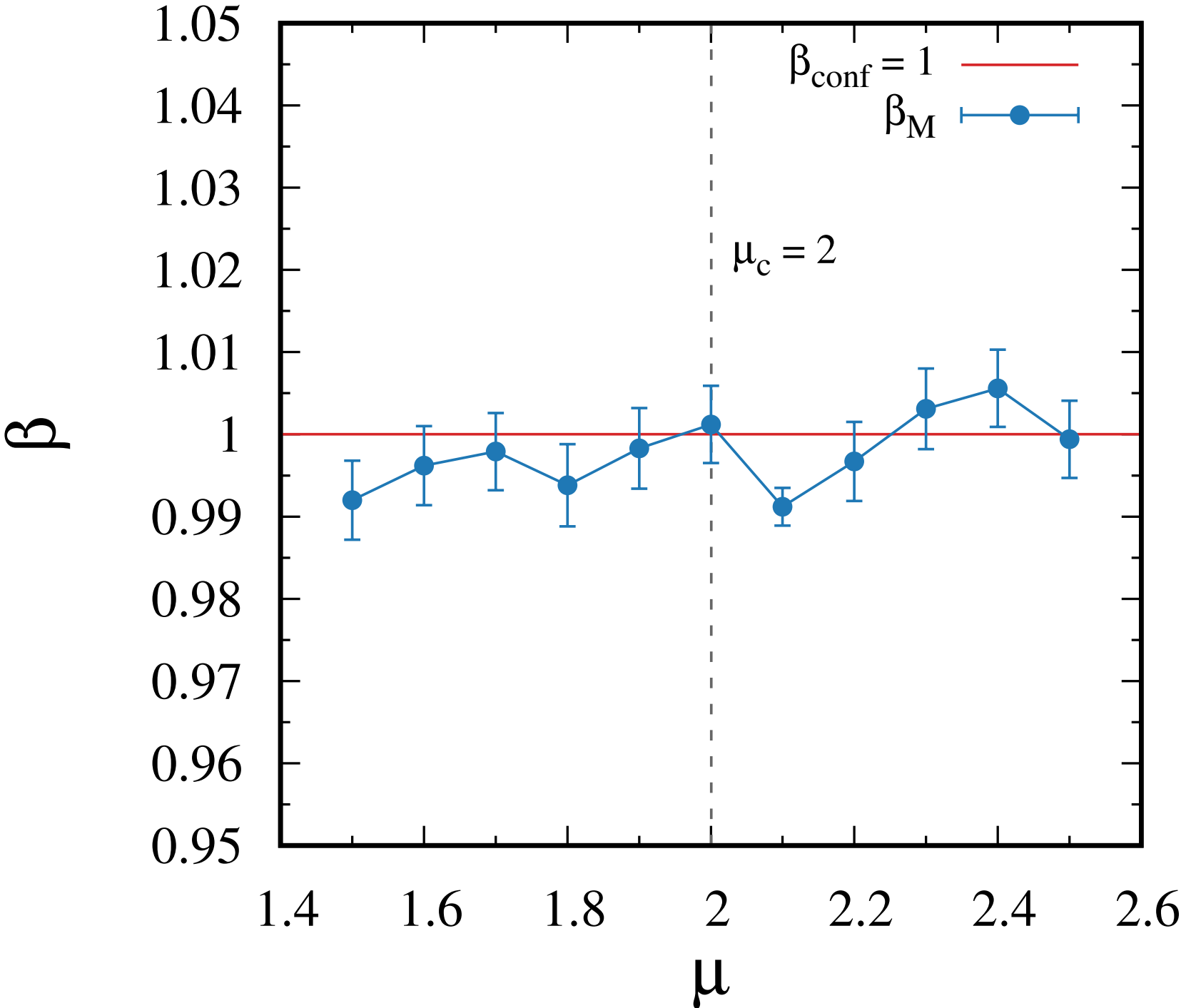
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Double Well Matrix Model

$$Z = \int dM \exp \left[-N \operatorname{Tr} \left(-\frac{\mu}{2} M^2 + \frac{1}{4} M^4 \right) \right] \quad M : \text{Hermitian}$$



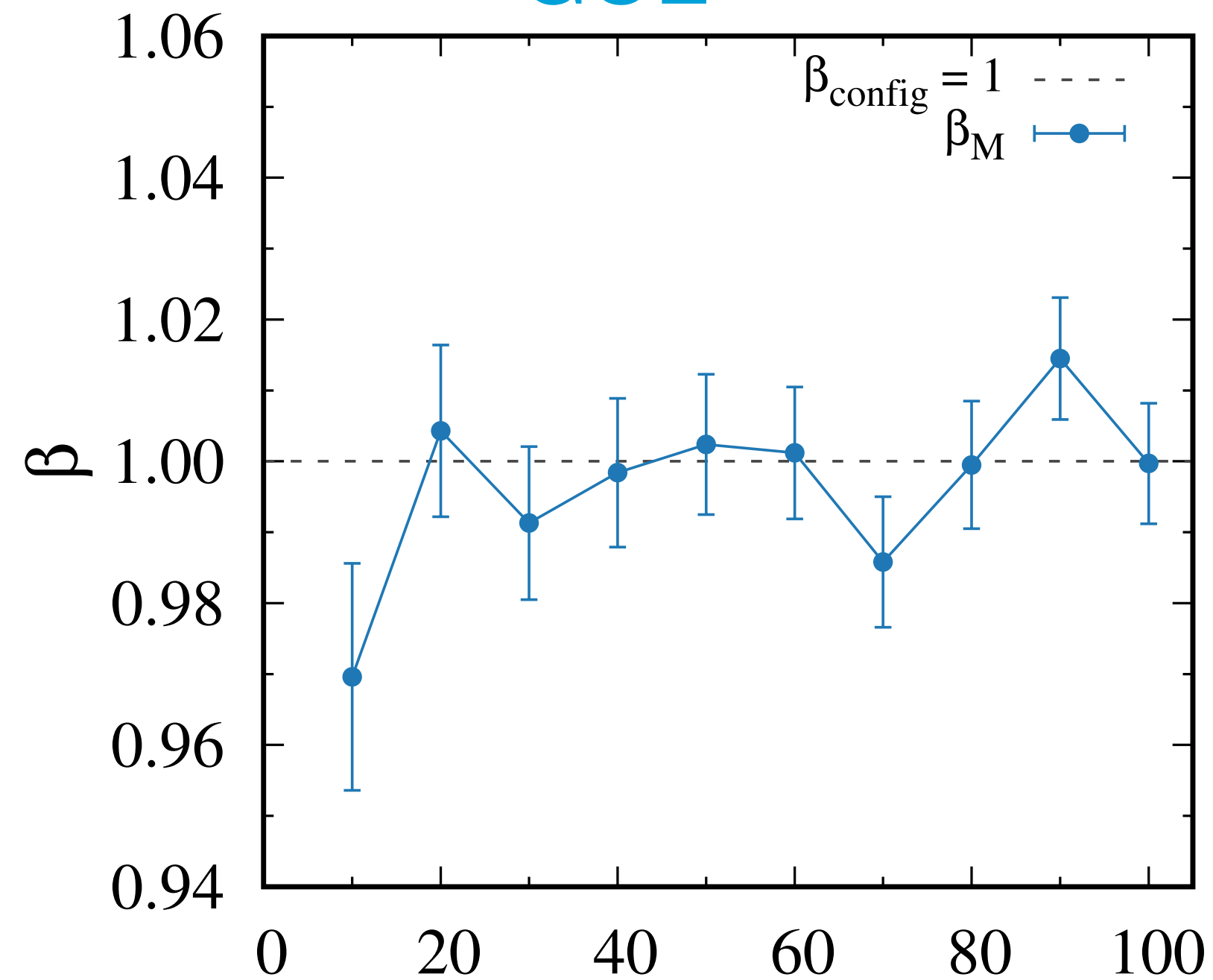
Gaussian Matrix Ensembles

- Notice relative closeness of scaling exponent for anisotropic and isotropic part in GWW(≈ -0.65) and double well matrix model(≈ -0.6).
- We want to check, how this exponent behaves for non-interacting models.
- Partition functions for these random matrix ensembles can be written as,

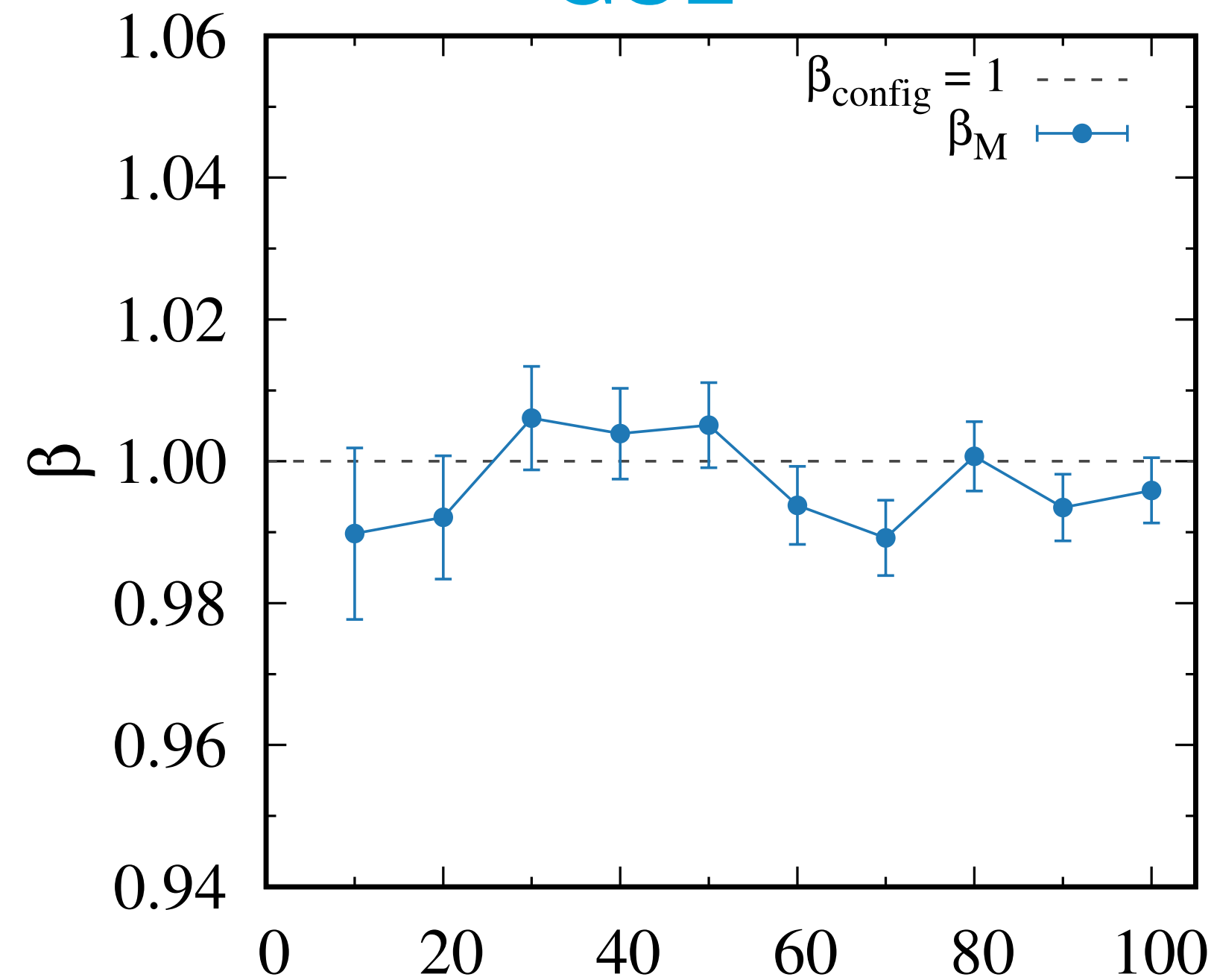
$$Z = \int \prod_{i=1}^N d\lambda_i e^{-S(\lambda)}, \quad S(\lambda) = \frac{1}{2} \sum_{i=1}^N \lambda_i^2 - \gamma \sum_{i < j} \log |\lambda_i - \lambda_j|.$$

$$\gamma = \begin{cases} 1, & \text{GOE,} \\ 2, & \text{GUE,} \\ 4, & \text{GSE.} \end{cases}$$

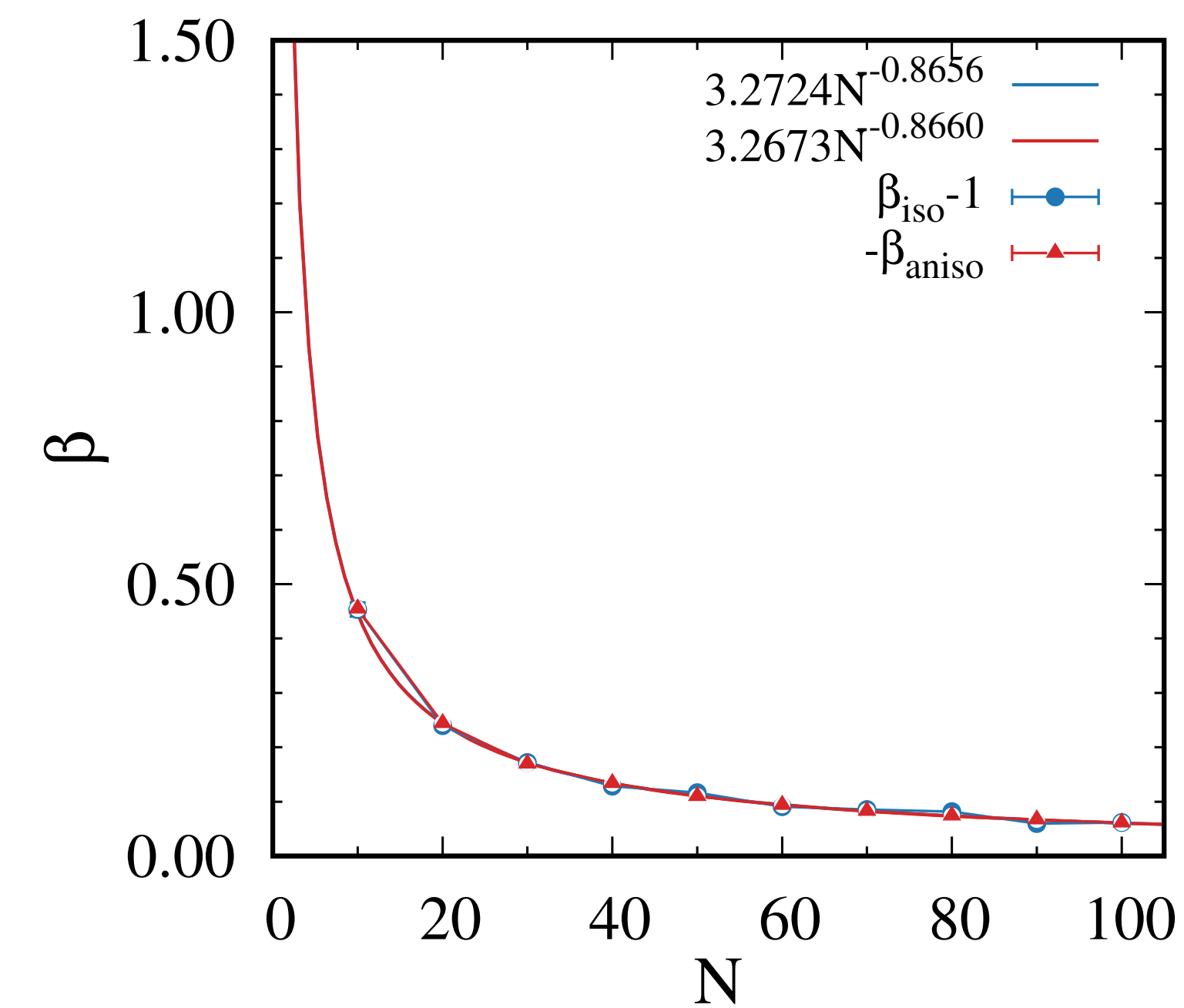
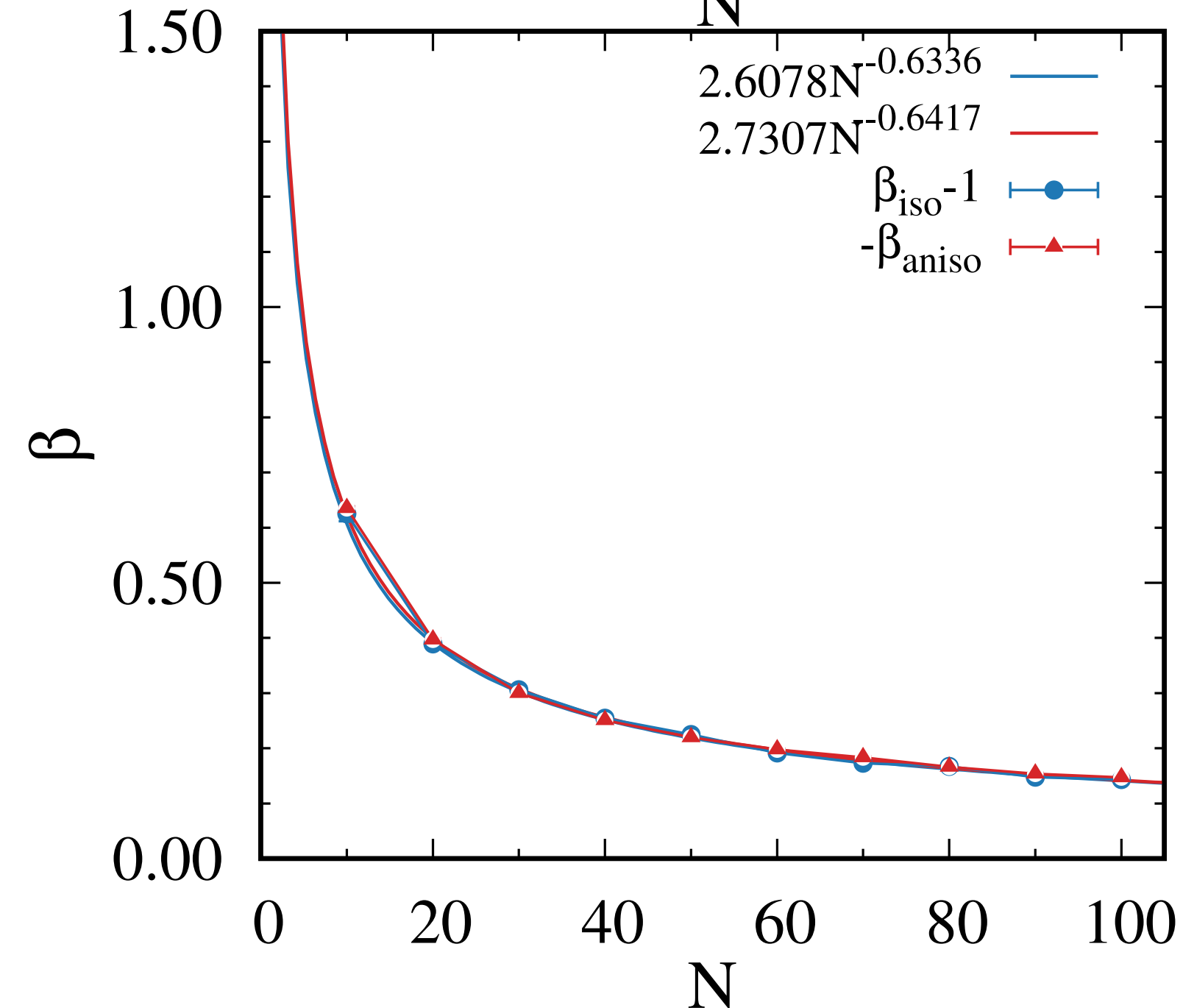
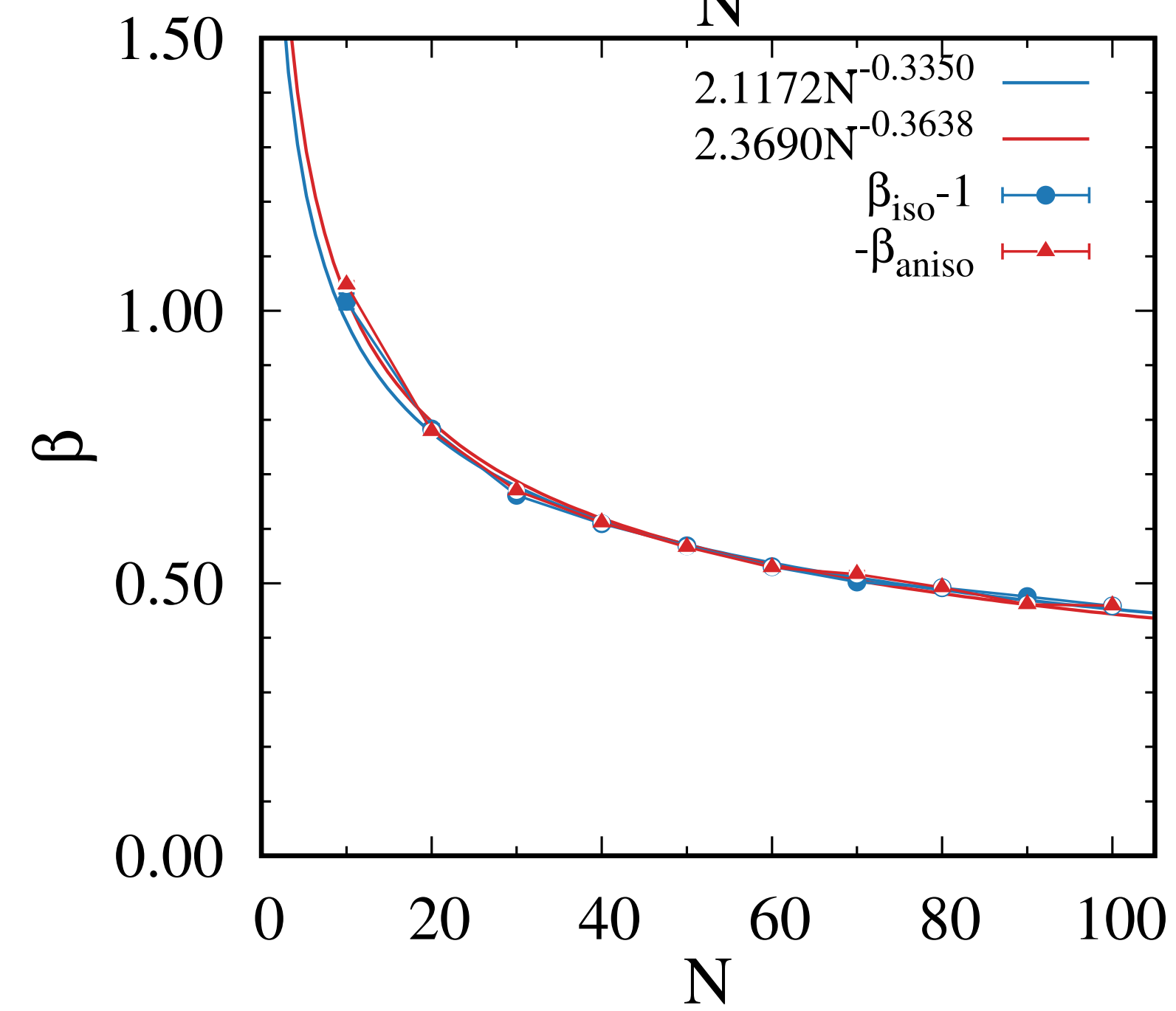
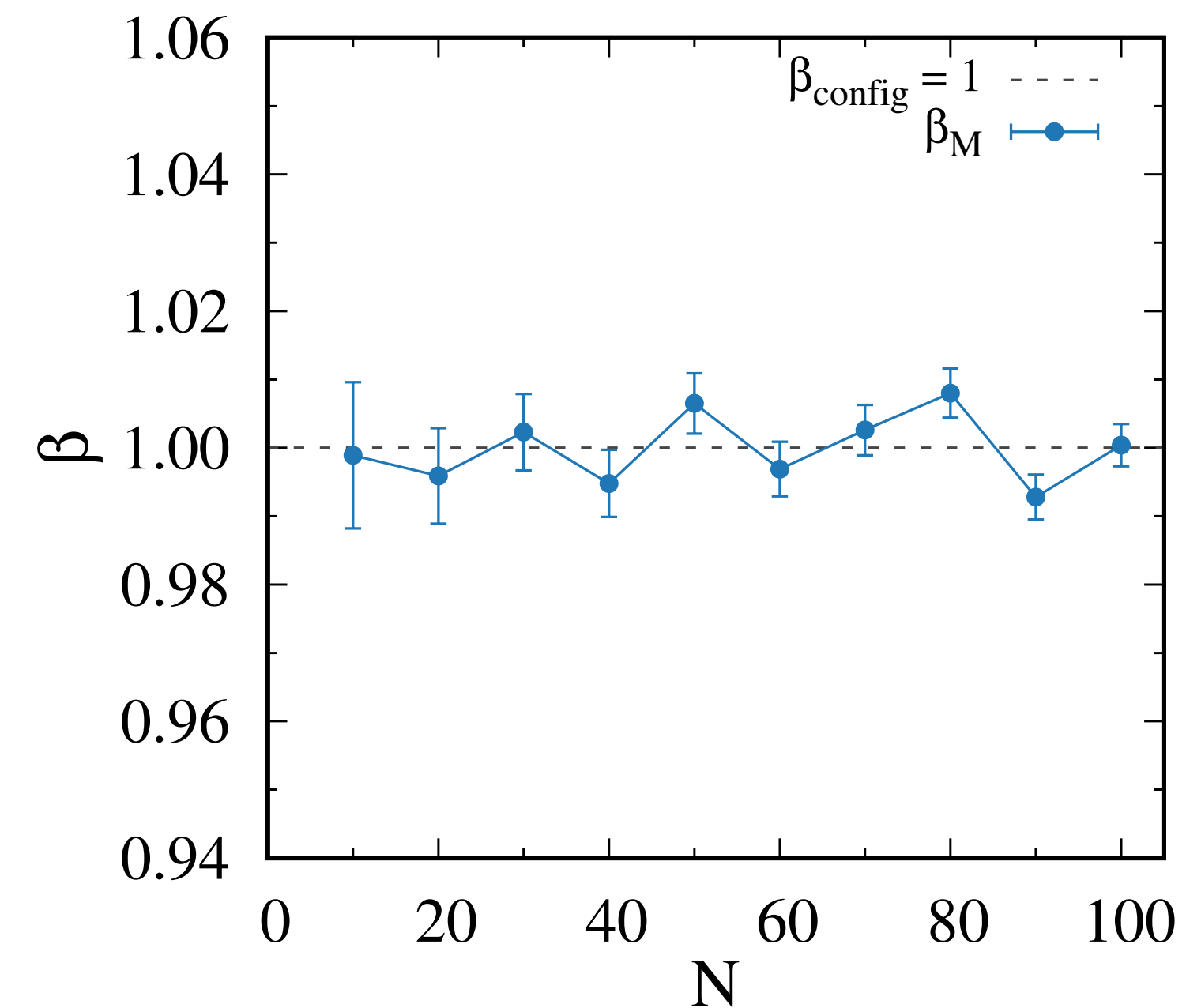
GOE



GUE



GSE



$$\beta_{\text{iso}} - 1 = A_{\text{iso}} N^{B_{\text{iso}}}$$

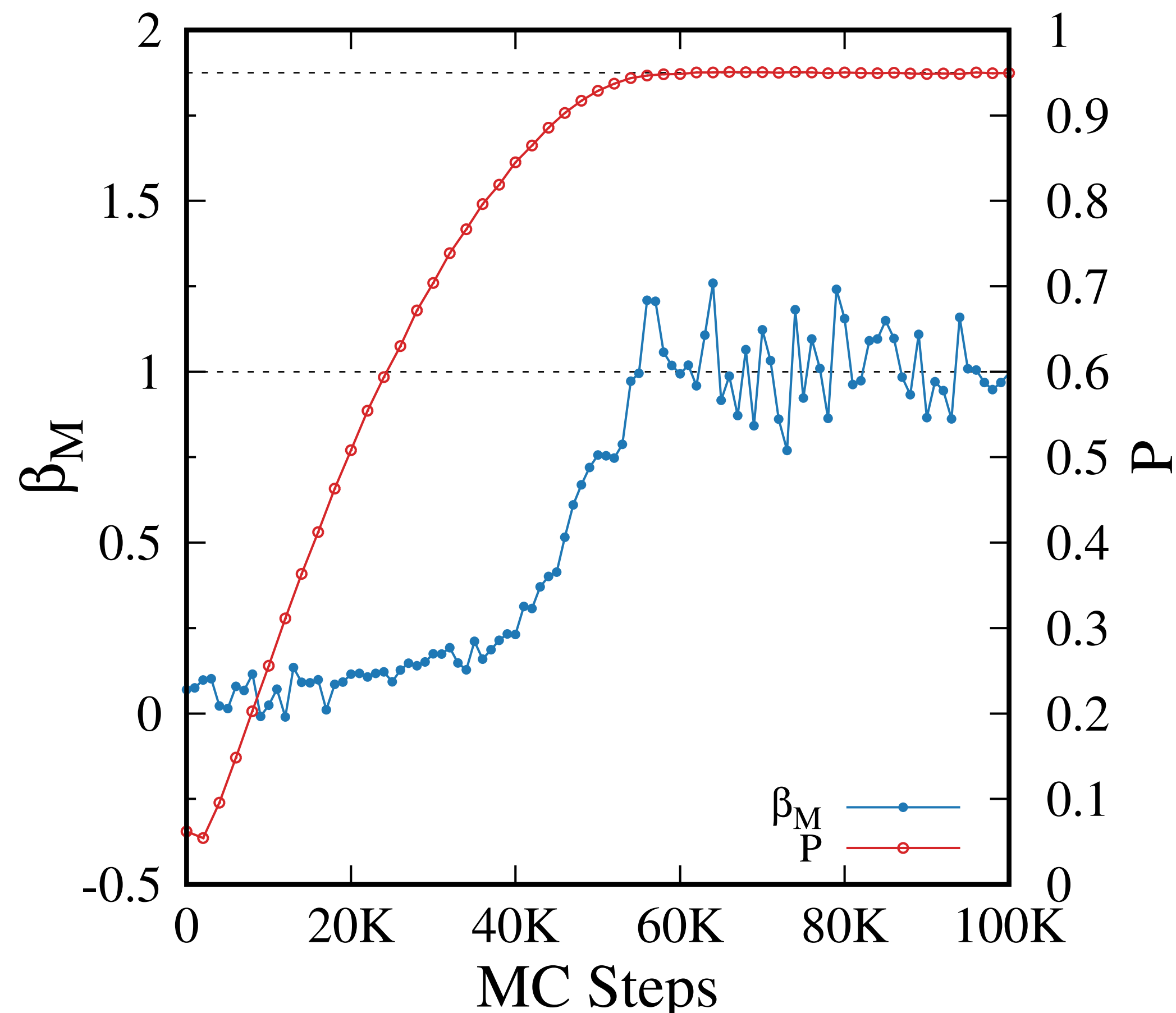
$$-\beta_{\text{aniso}} = A_{\text{aniso}} N^{B_{\text{aniso}}}$$

Model	B_{iso}	B_{aniso}
GOE	$-0.3350(92)$	$-0.3638(93)$
GUE	$-0.6336(82)$	$-0.6417(90)$
GSE	$-0.8656(228)$	$-0.8660(50)$
Double Well	-0.59 to -0.63	-0.60 to -0.61
GWW	-0.64 to -0.67	-0.65 to -0.68

- The finite N scaling exponent fits the relation $\beta_{\text{iso}} - 1 \simeq -\beta_{\text{aniso}}$ across matrix ensembles.
- It does not differentiate between interacting and non-interacting models.
- It solely depends on underlying model.

Configurational Temperature as a Monte Carlo Diagnostic

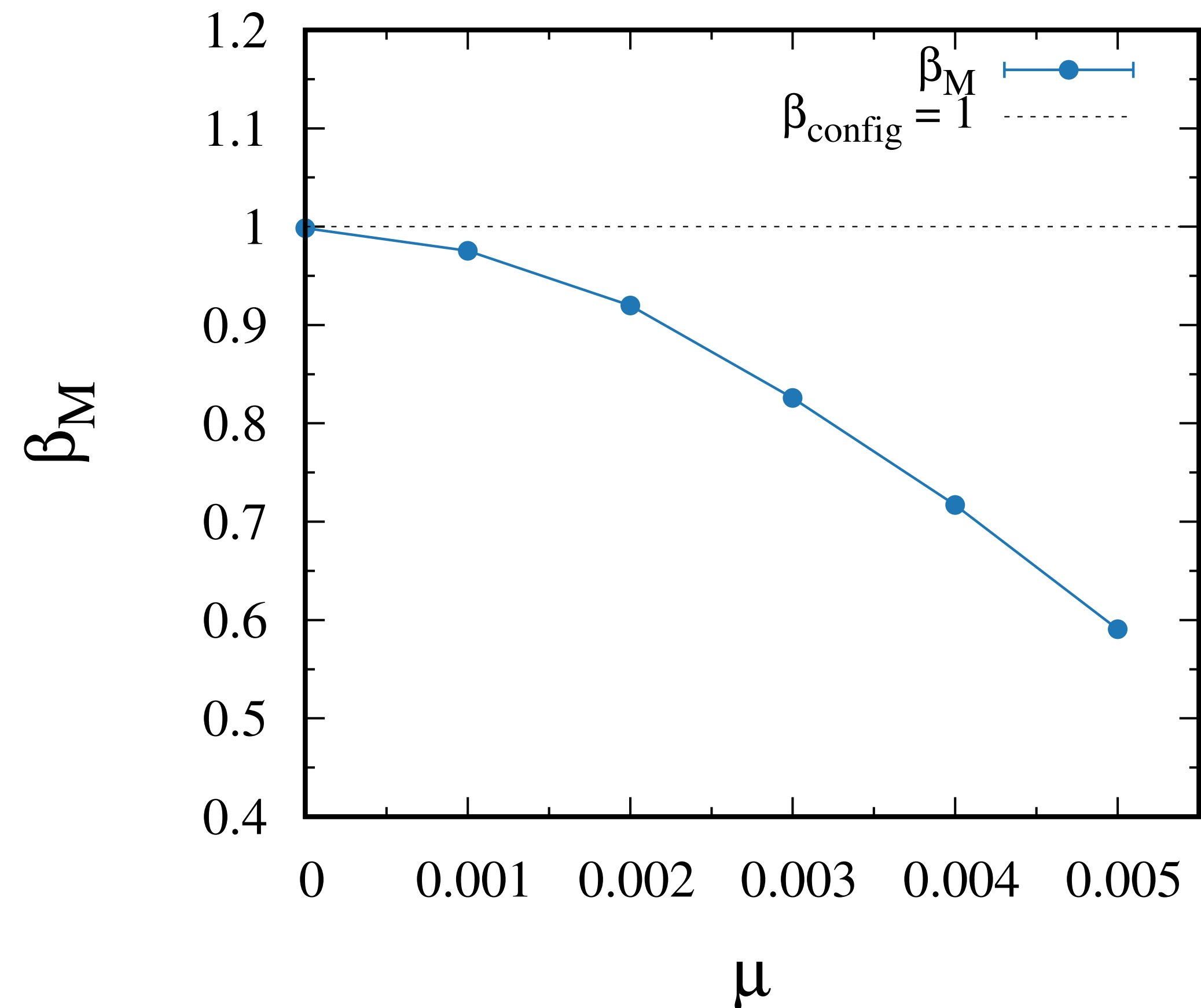
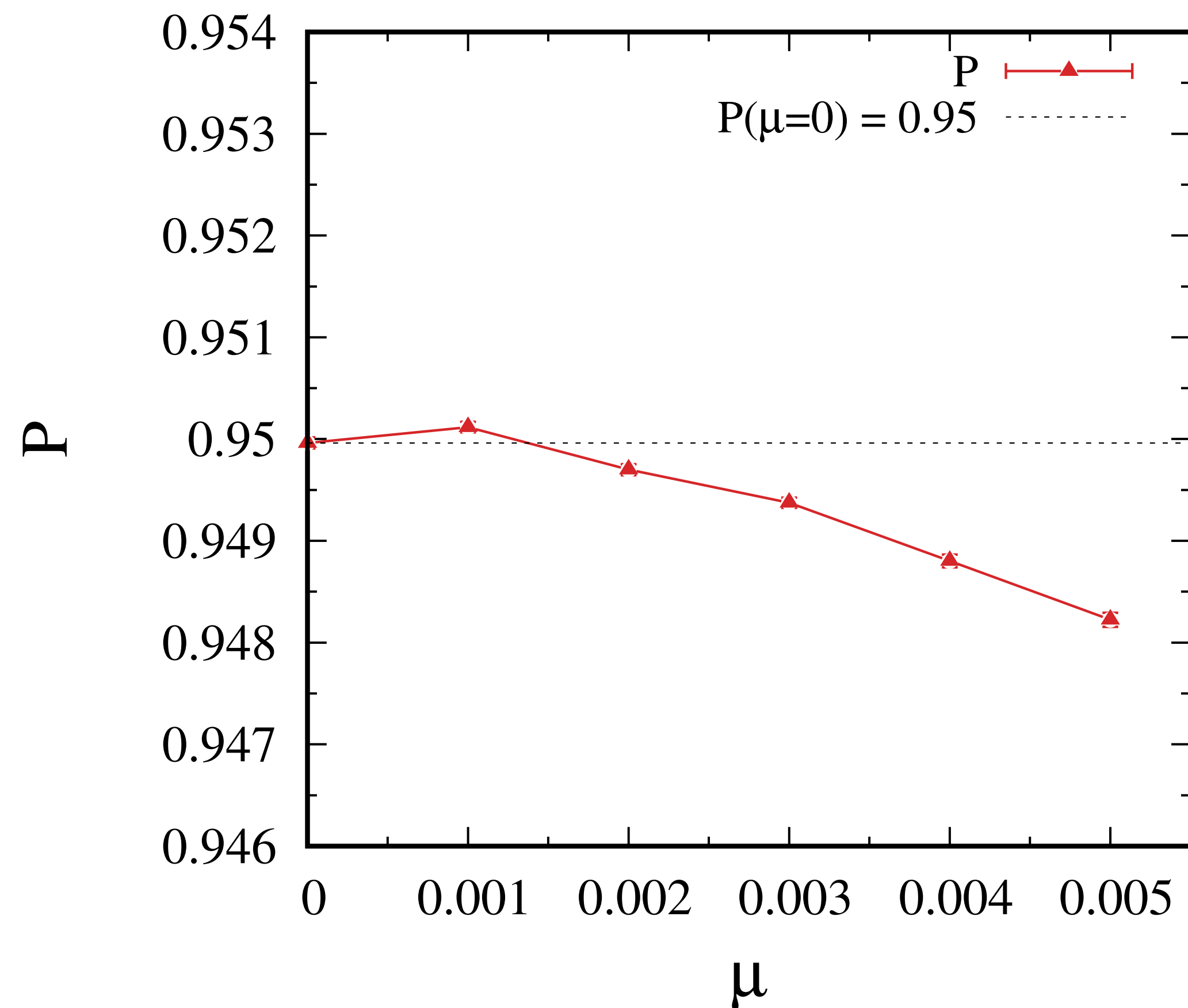
Thermalisation



- Starting from a disordered state, evolution of Polyakov loop shows relatively quick thermalisation.
- β_M approaches the expected value of one, more gradually.
- As simulation proceeds, the estimator becomes consistent with exact identity.
- This highlights sensitivity of the estimator.

Detection of Biased Sampling

- We introduce bias into Metropolis proposal as, $\theta_i \rightarrow \theta_i + \delta + \mu$. $\delta \in [-\epsilon, \epsilon]$
- Polyakov loop exhibits only a modest response, whereas configurational estimator demonstrates high sensitivity to violations of detailed balance.



Summary

- Configurational Temperature Estimator follows from an exact Schwinger-Dyson identity.
- For correctly sampled ensembles, the estimator satisfies the identity $\beta_{config} = 1$.
- Cancellation pattern of isotropic and anisotropic sectors of the estimator is robust across all models, but does not have universal scaling exponent.
- Can be used as a diagnostic tool for Monte Carlo simulation correctness of matrix models.

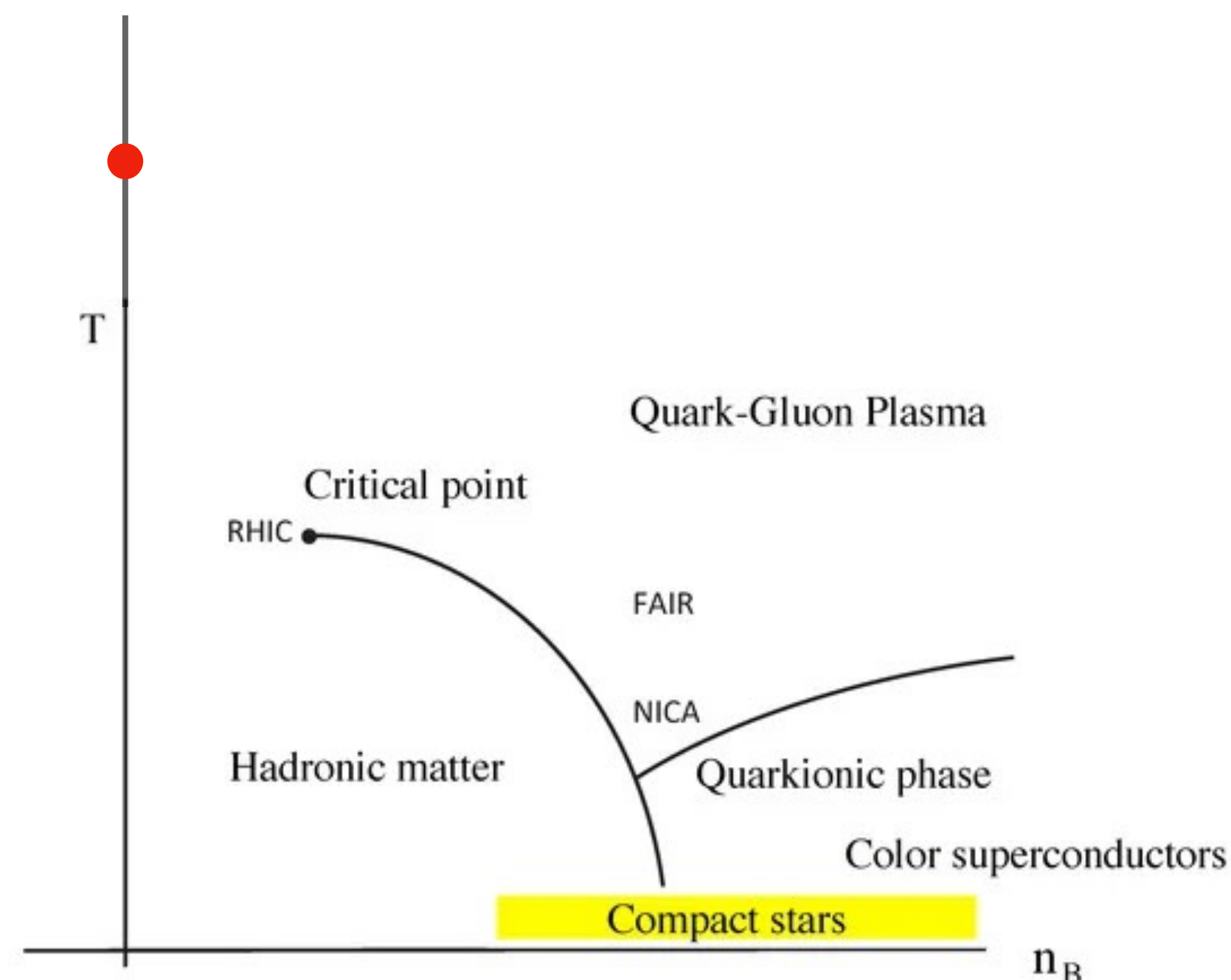
Metastable states in $2 + 1$ flavor QCD

Sanatan Digal, Prasad Hegde, VM

Outline

- Role of Z_3 symmetry in pure SU(3) gauge theory and confinement-deconfinement transition.
- Effect of including dynamical quarks on Z_3 symmetry.
- Briefly describe simulation details to observe metastable states in deconfined phase of QCD.
- Results
- Discussion

- Study of QCD, fundamental theory of strong interactions, is key to understanding how matter behaves under extreme conditions.
- In heavy ion collisions, hadrons melt and quark-gluon plasma is formed; which is the most perfect fluid known to us.



- In this study, we explore metastable states related to Z_3 symmetry around the region shown by red dot in the schematic phase diagram.

*Credit: *Particles* 2023, 6(3), 713

- Here, we take a small review of Z_3 symmetry in pure $SU(3)$ theory.

- For pure $SU(3)$ gauge theory at finite temperature T

$$\mathcal{Z} = \int D[A] e^{-S_G}$$

$$S_G[A] = \int_0^\beta d\tau \int_V d^3x \left\{ \frac{1}{4} F_{\mu\nu}^a F_{\mu\nu}^a \right\}, \quad F_{\mu\nu}^a = \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + g f^{abc} A_\mu^b A_\nu^c$$

- Path integral is over all A satisfying $A(\mathbf{x},0) = A(\mathbf{x},\beta)$
- As we are interested in gauge fields coupled to matter fields in the fundamental representation, then gauge transformations are classified by the center

$$Z_3 \in SU(3). \quad A' = V A V^{-1} + \frac{i}{g} V \partial V^{-1}, \quad V(\mathbf{x},\beta) = z V(\mathbf{x},0), \quad z \in Z_3.$$

- Wilson line: $W(x_1, x_2) = P \exp \left[ig \int_{x_1}^{x_2} dx \cdot A \right]$
- Which transforms as $W(x_1, x_2) \longrightarrow V(x_1)W(x_1, x_2)V(x_2)^{-1}$
- Polyakov loop(PL), which is a closed Wilson line in temporal direction, is not invariant under certain Z_3 gauge transformations:

$$L(\mathbf{x}) = \frac{1}{N} \text{Tr} \{ W(\mathbf{x}, 0; \mathbf{x}, \beta) \}$$

$$V(\mathbf{x}, \beta) = zV(\mathbf{x}, 0) \implies L(\mathbf{x}) \longrightarrow zL(\mathbf{x})$$

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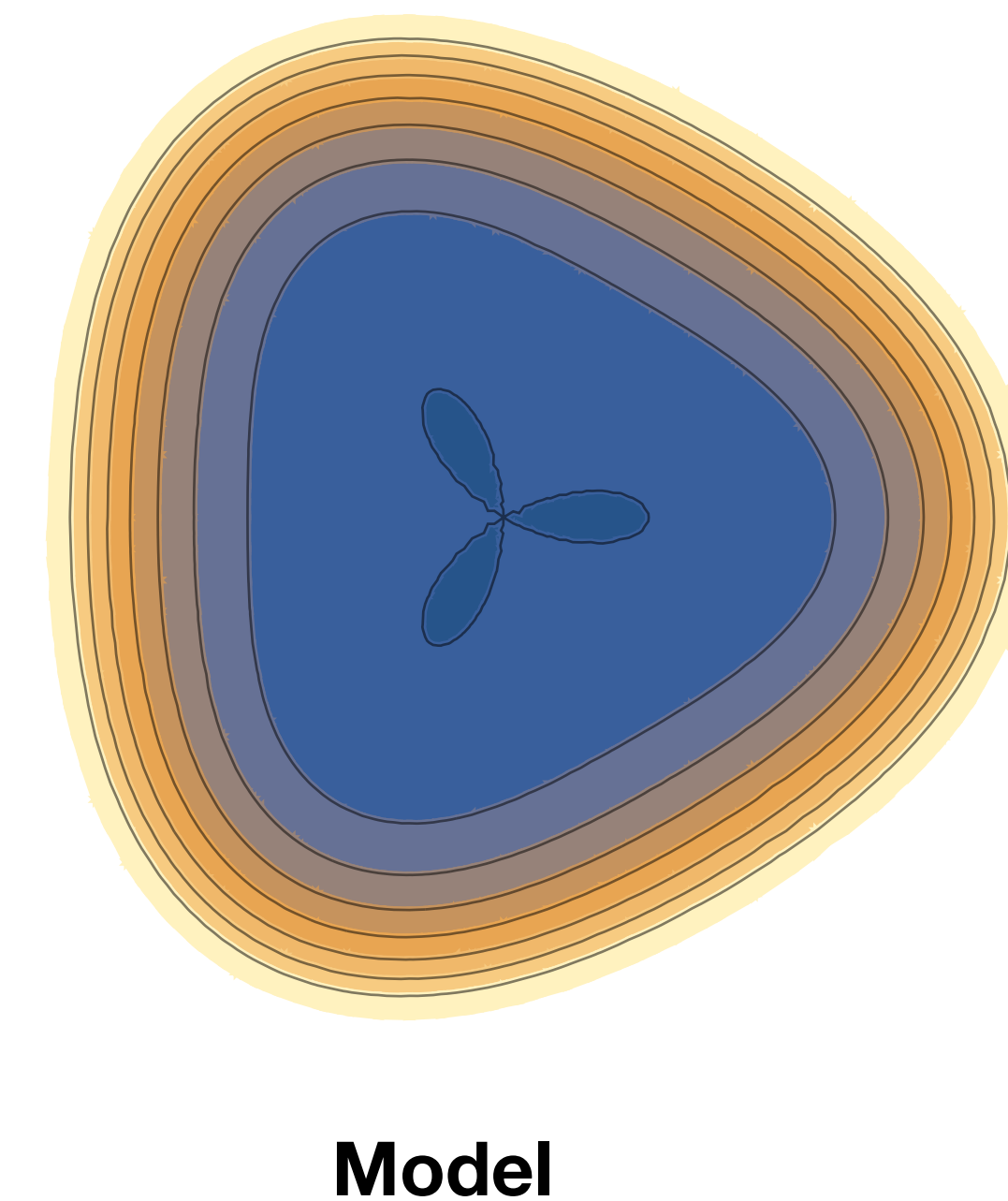
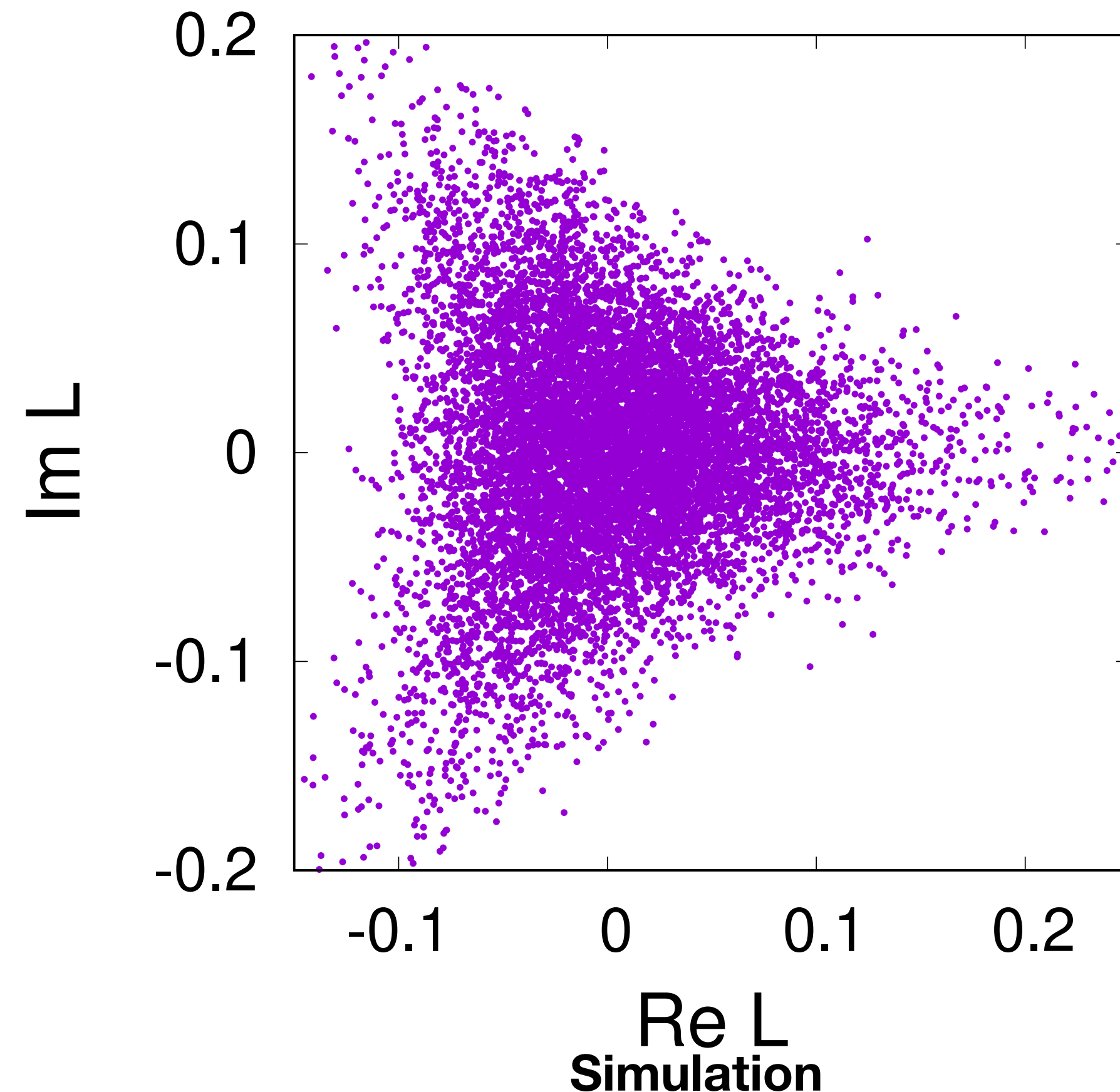
$$L(\mathbf{x}) = \frac{1}{N} \text{Tr} \{ W(\mathbf{x}, 0; \mathbf{x}, \beta) \}$$

$$V(\mathbf{x}, \beta) = z V(\mathbf{x}, 0) \implies L(\mathbf{x}) \longrightarrow z L(\mathbf{x}) \quad | \langle L \rangle |^2 \approx e^{-F_{q\bar{q}}/T}$$

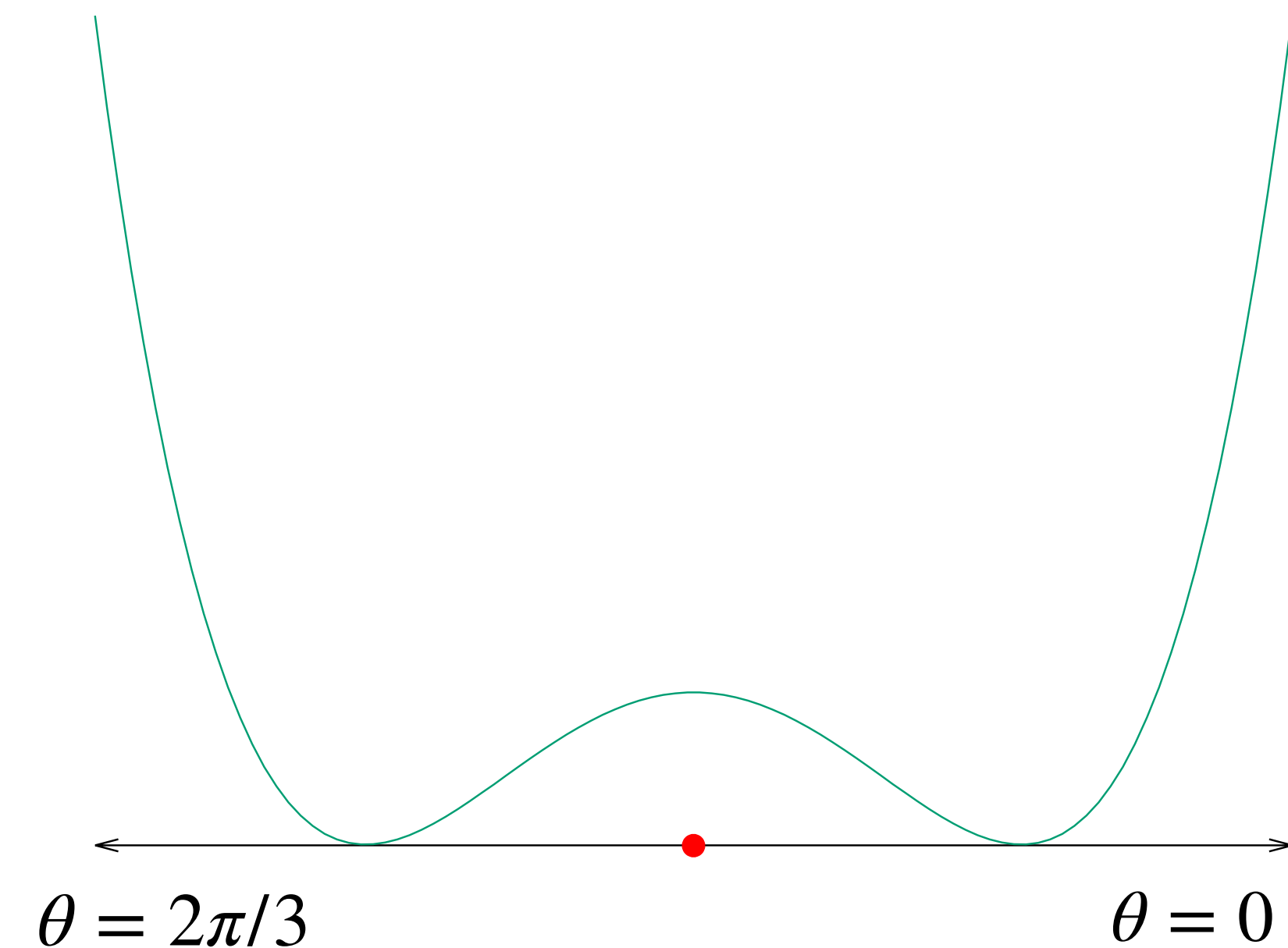
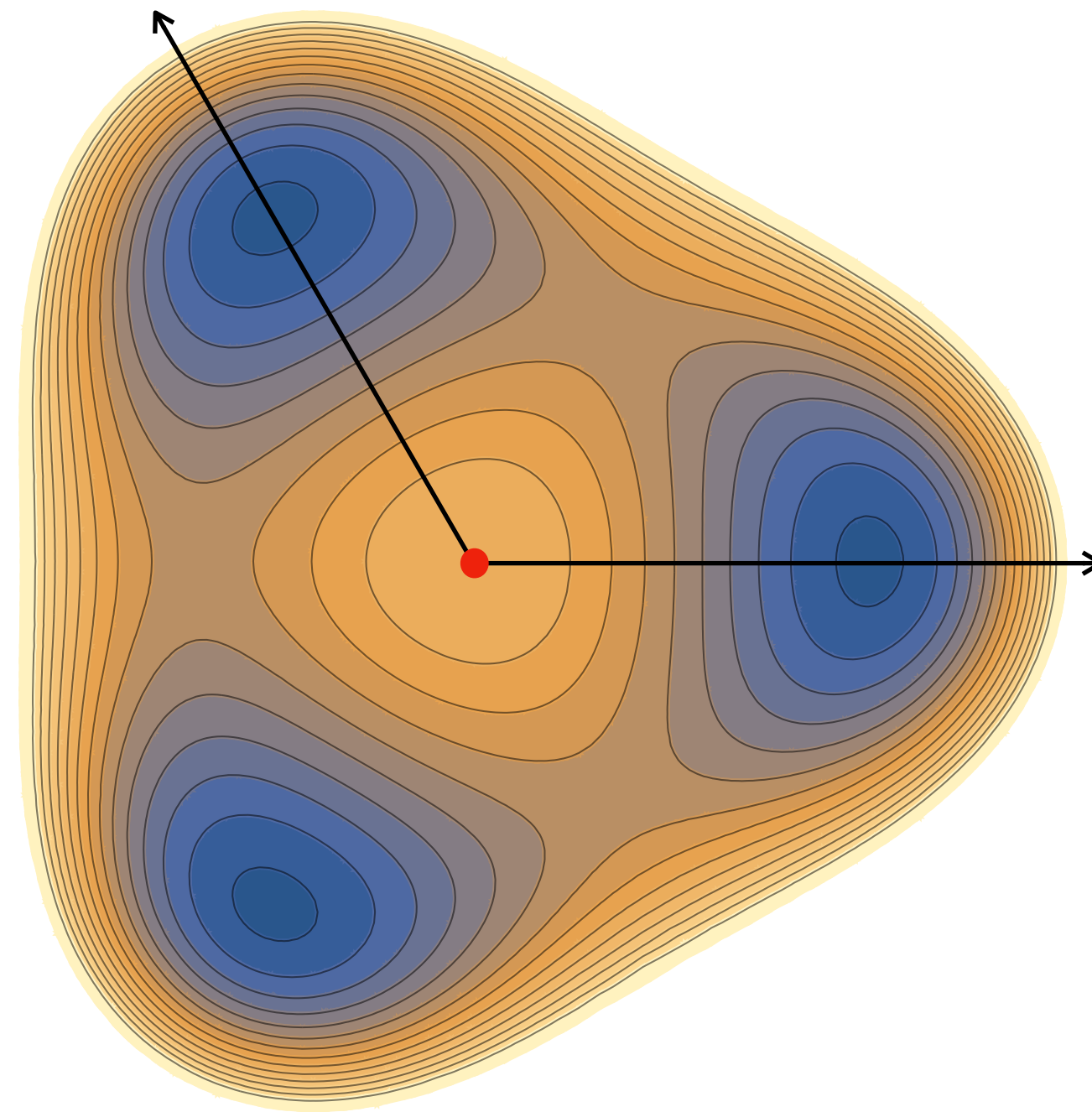
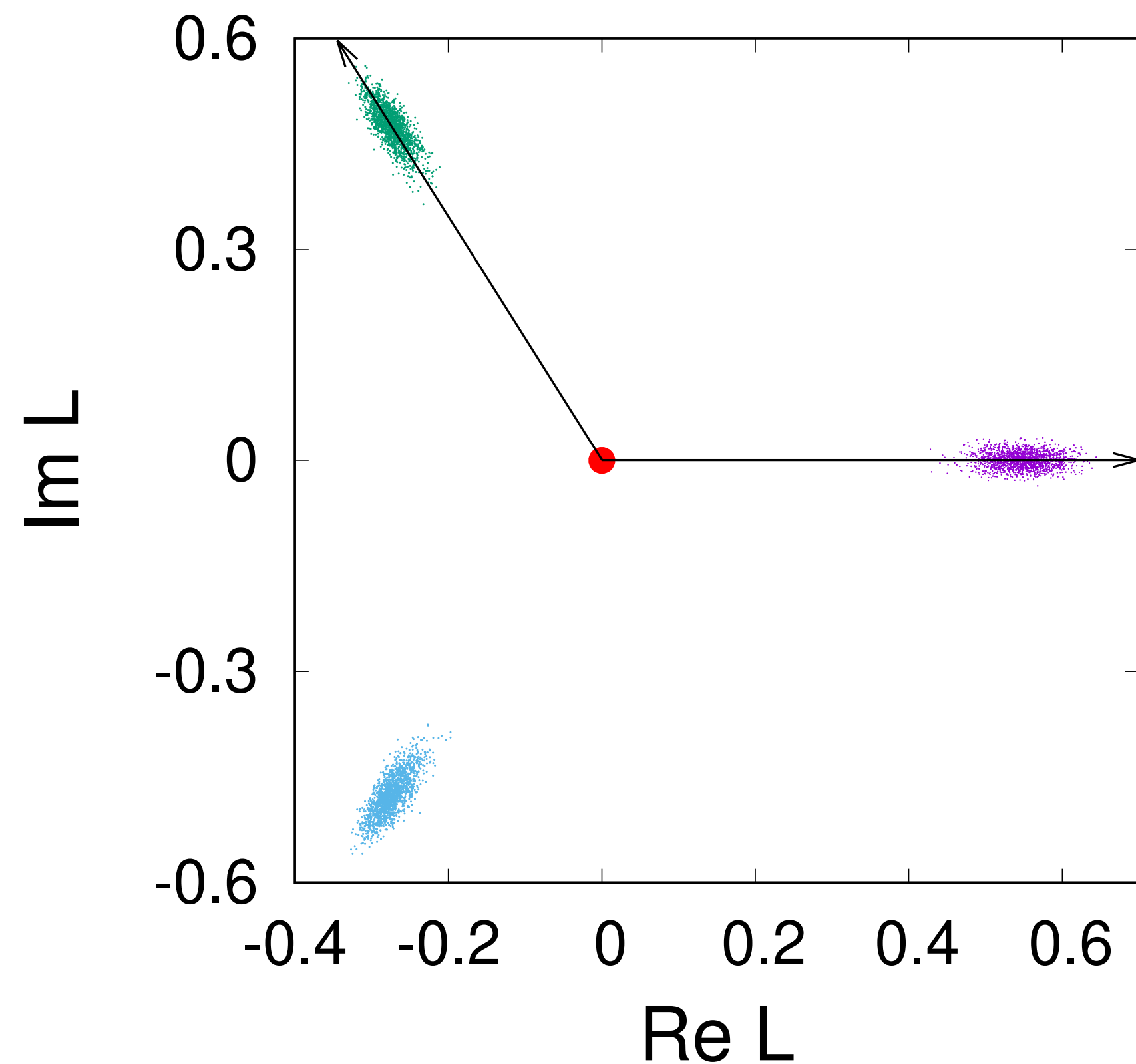
- PL acts as an order parameter for confinement-deconfinement(CD) transition, associated with spontaneous breaking of Z_3 symmetry.

- In case of pure $SU(3)$ gauge theory, the effective potential in the confined phase could be qualitatively estimated in accordance with underlying Z_3 symmetry

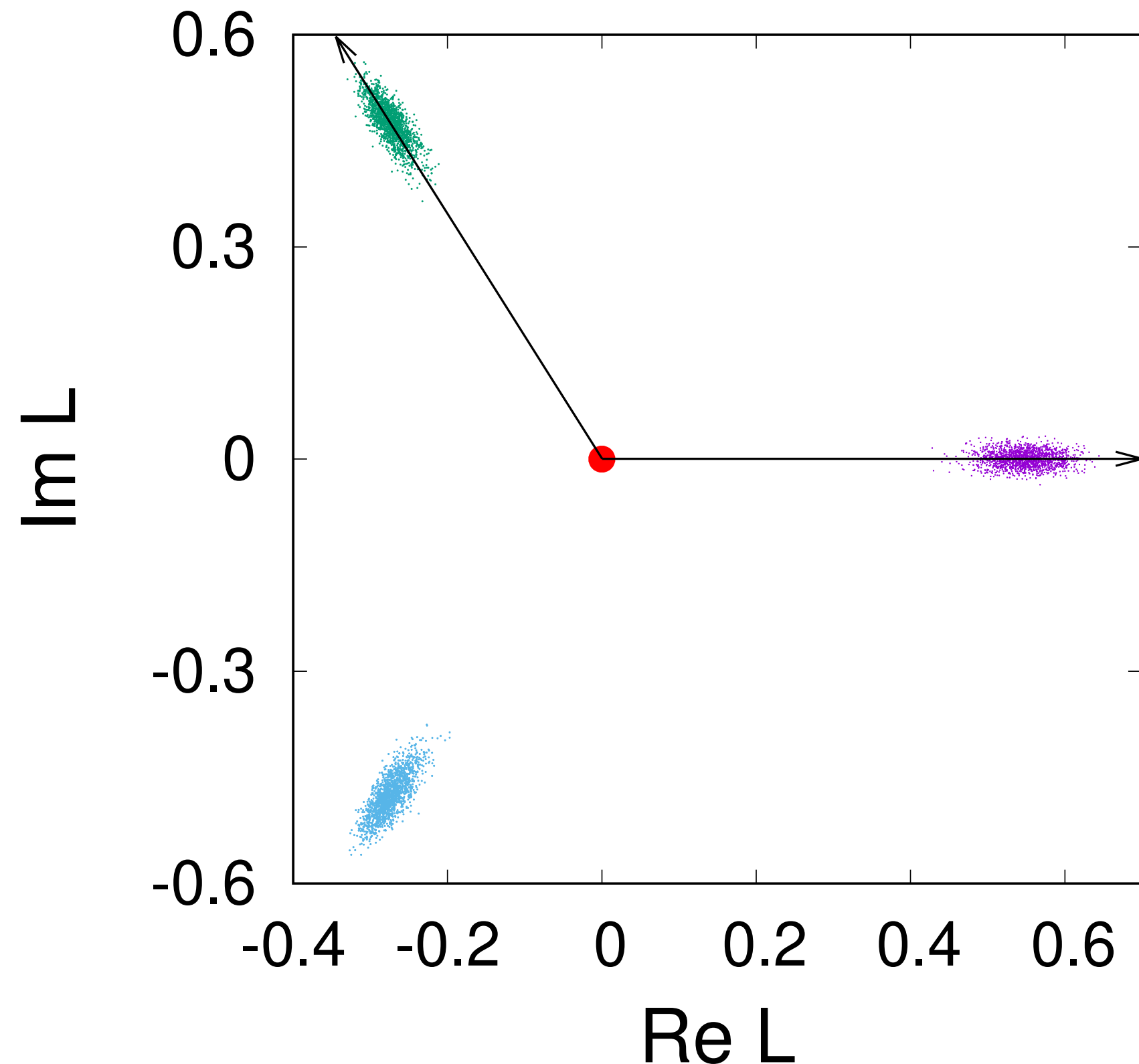
$$\frac{{}^*U(L, \bar{L}, T)}{T^4} = -b_0(T)\bar{L}L - b_1(L^3 + \bar{L}^3) + b_2(\bar{L}L)^2$$



- Whereas in the deconfined phase, we get Z_3 related degenerate states.
- The left diagram is actual polyakov loop distribution from pure gauge theory simulations. The middle plot of potential is from effective field model.
- Schematically, potential along the line in the middle figure would look like curve on the right



- Whereas in the deconfined phase, we get Z_3 related degenerate states.
- The left diagram is actual polyakov loop distribution from pure gauge theory simulations. The middle plot of potential is from effective field model.
- Schematically, potential along the line in the middle figure would look like curve on the right



- Due to the barrier separating Z_3 vacua, it is not possible to observe all three states in a single Monte Carlo run. One needs to consider different initial conditions to observe them.
- Perturbative studies show that barrier height between different spontaneously broken vacua increases with increase in temperature.

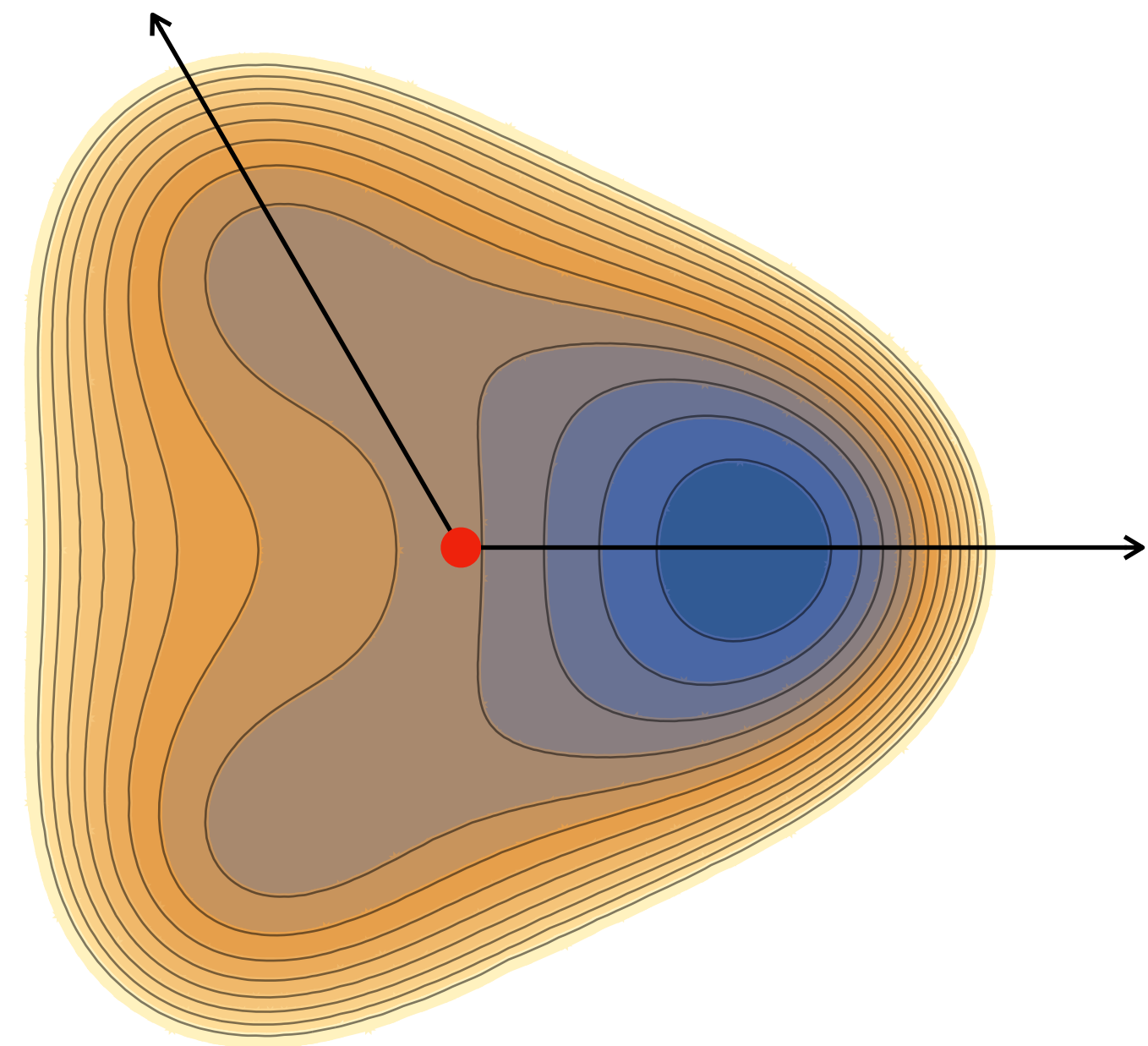
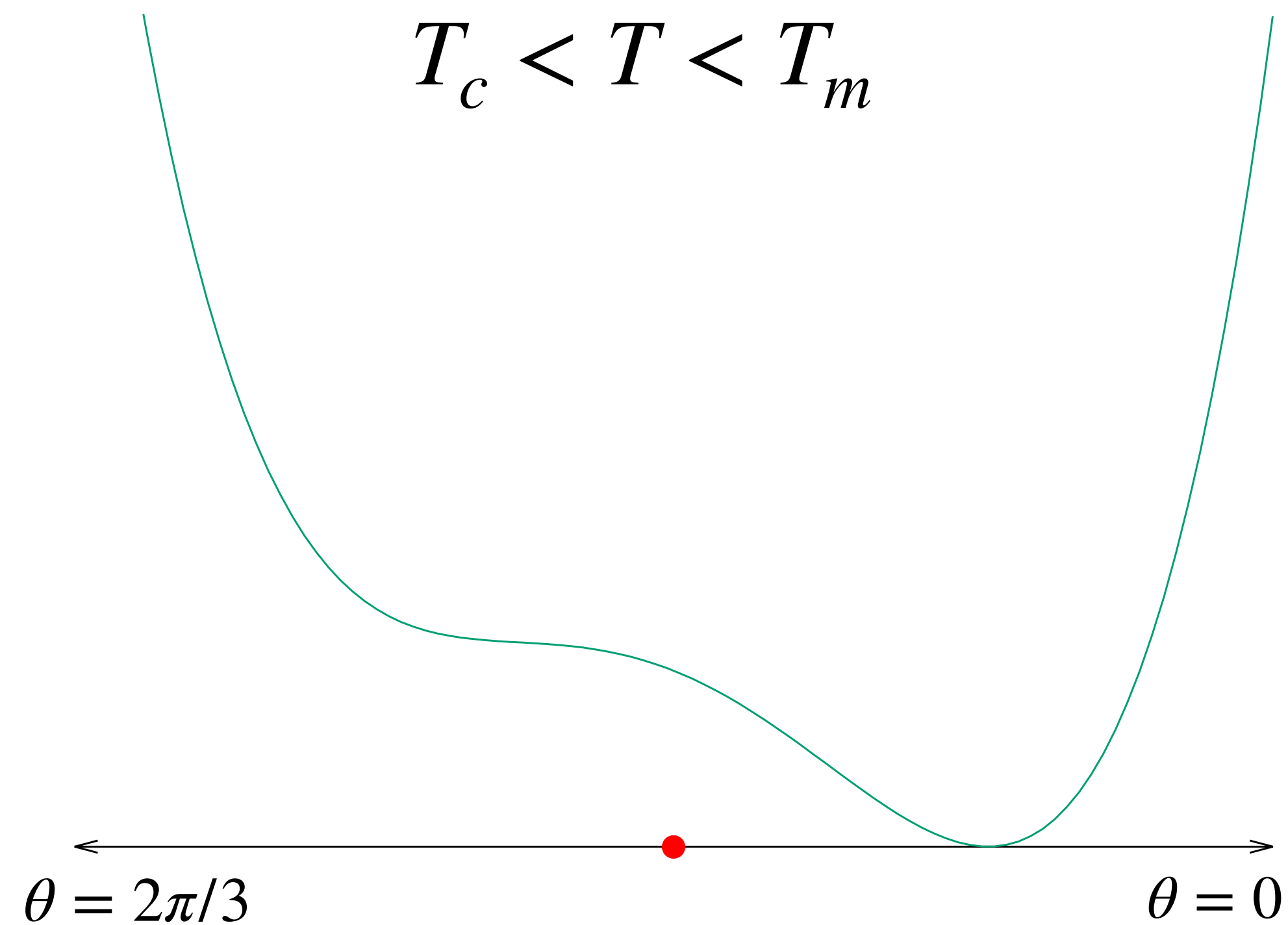
- In presence of fermions:

$$\mathcal{Z} = \int D[A] D[\psi] D[\bar{\psi}] e^{-S}, \quad S = S_G + S_F$$

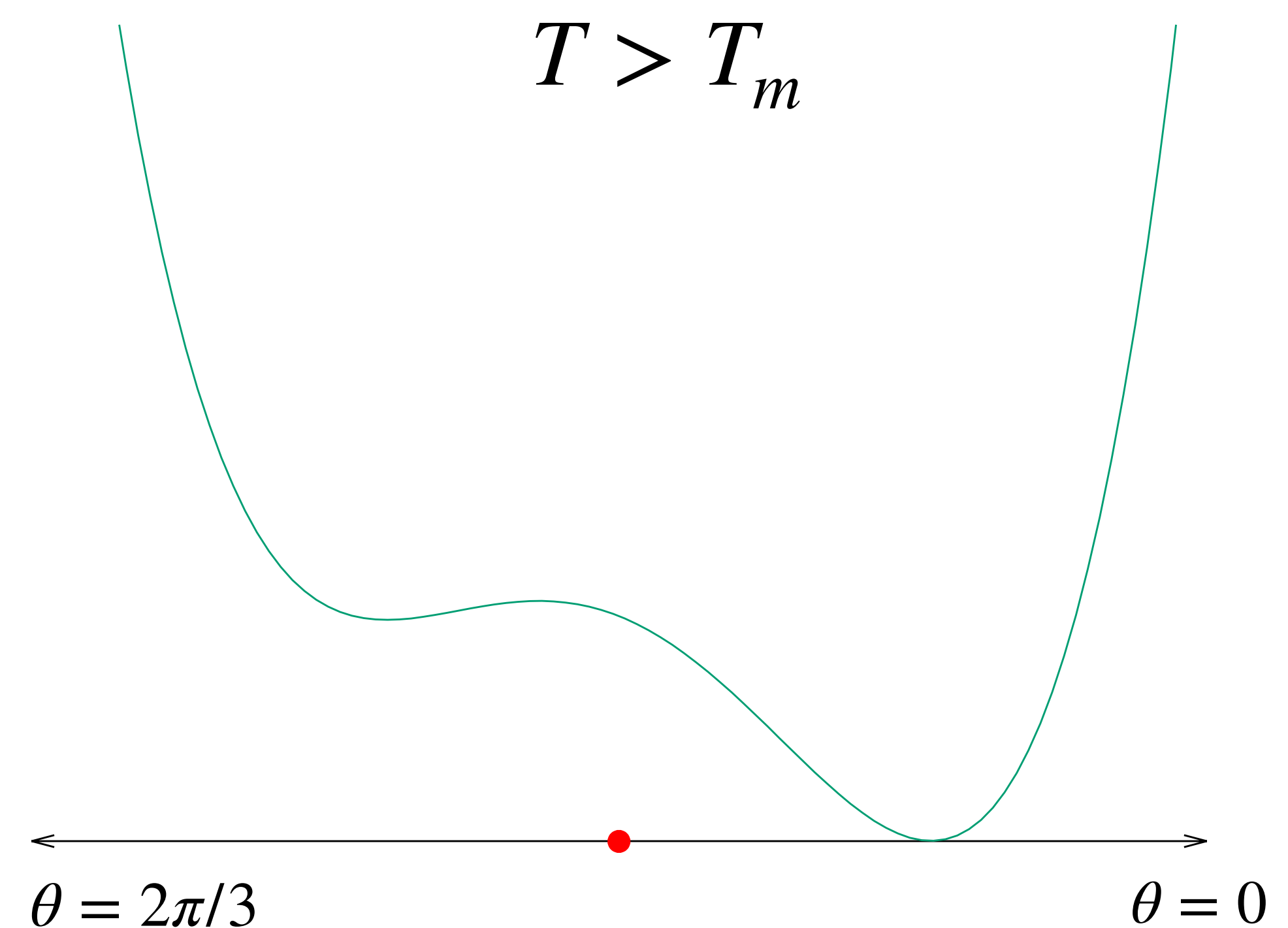
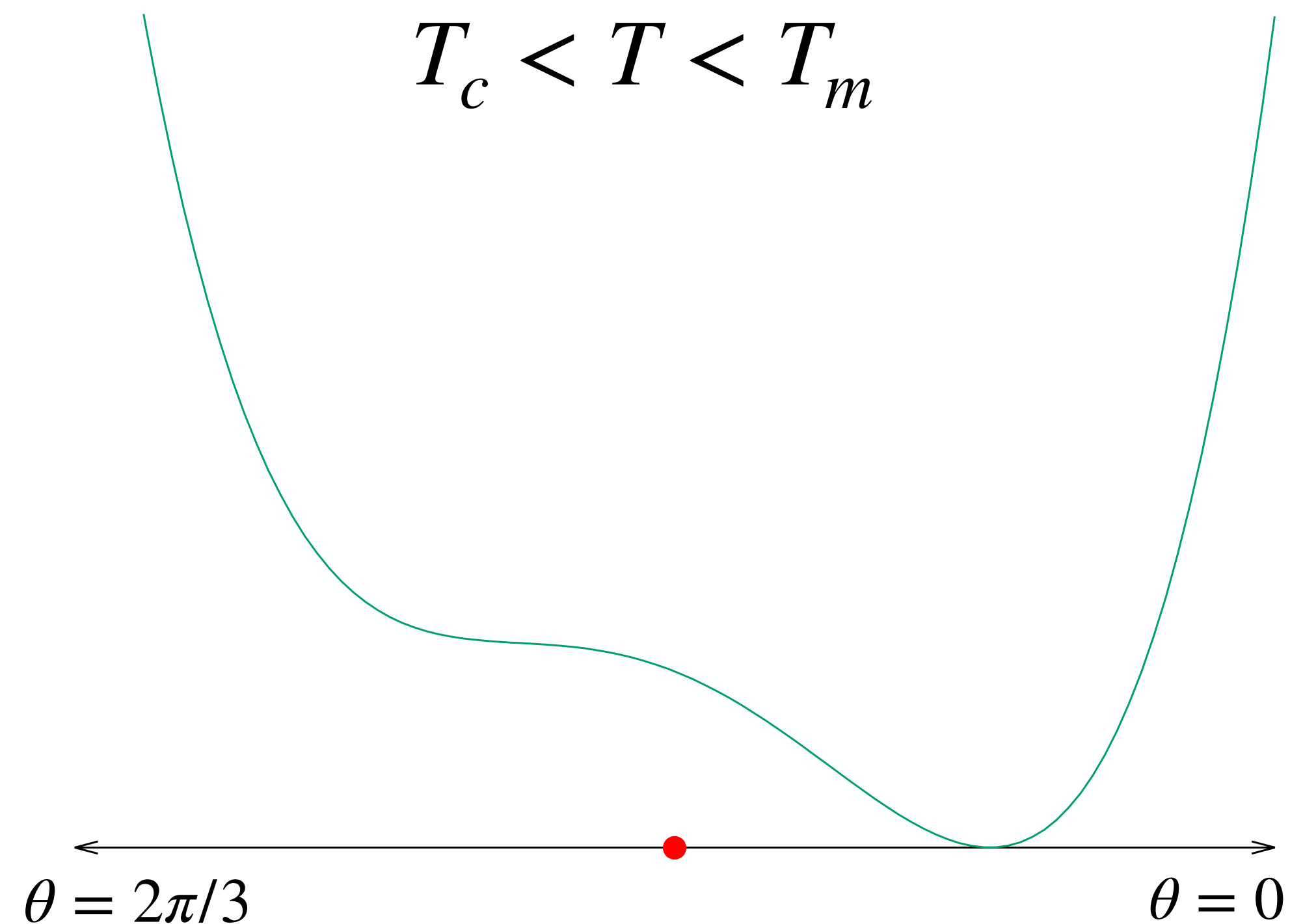
$$S_F[\psi, \bar{\psi}, A] = \int_0^\beta d\tau \int_V d^3x \left\{ \bar{\psi}(\gamma_\mu D_\mu + m)\psi \right\} \quad D_\mu = \partial_\mu - igA_\mu$$

- Path integral is over all ψ satisfying $\psi(\mathbf{x}, 0) = -\psi(\mathbf{x}, \beta)$
- Gauge transformations: $\psi(x) \longrightarrow V(x)\psi(x)$
- For transformations $V(\mathbf{x}, \beta) = zV(\mathbf{x}, 0)$, only identity element of Z_3 contributes to the partition function.
- So, L and zL do not contribute equally to the partition function, leading to explicit breaking of Z_3 symmetry. This makes states with PL phase $\theta = \pm 2\pi/3$ less probable.

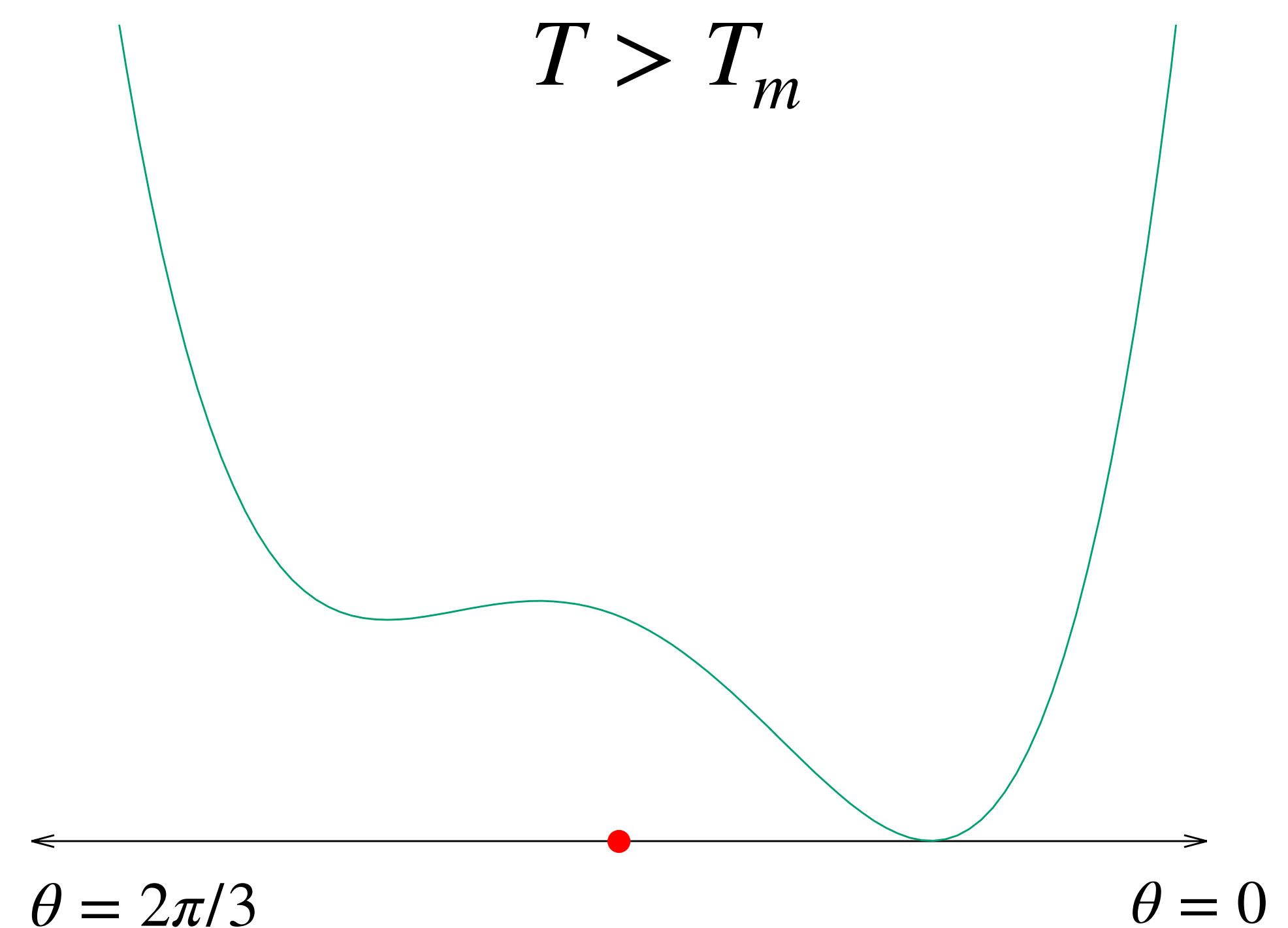
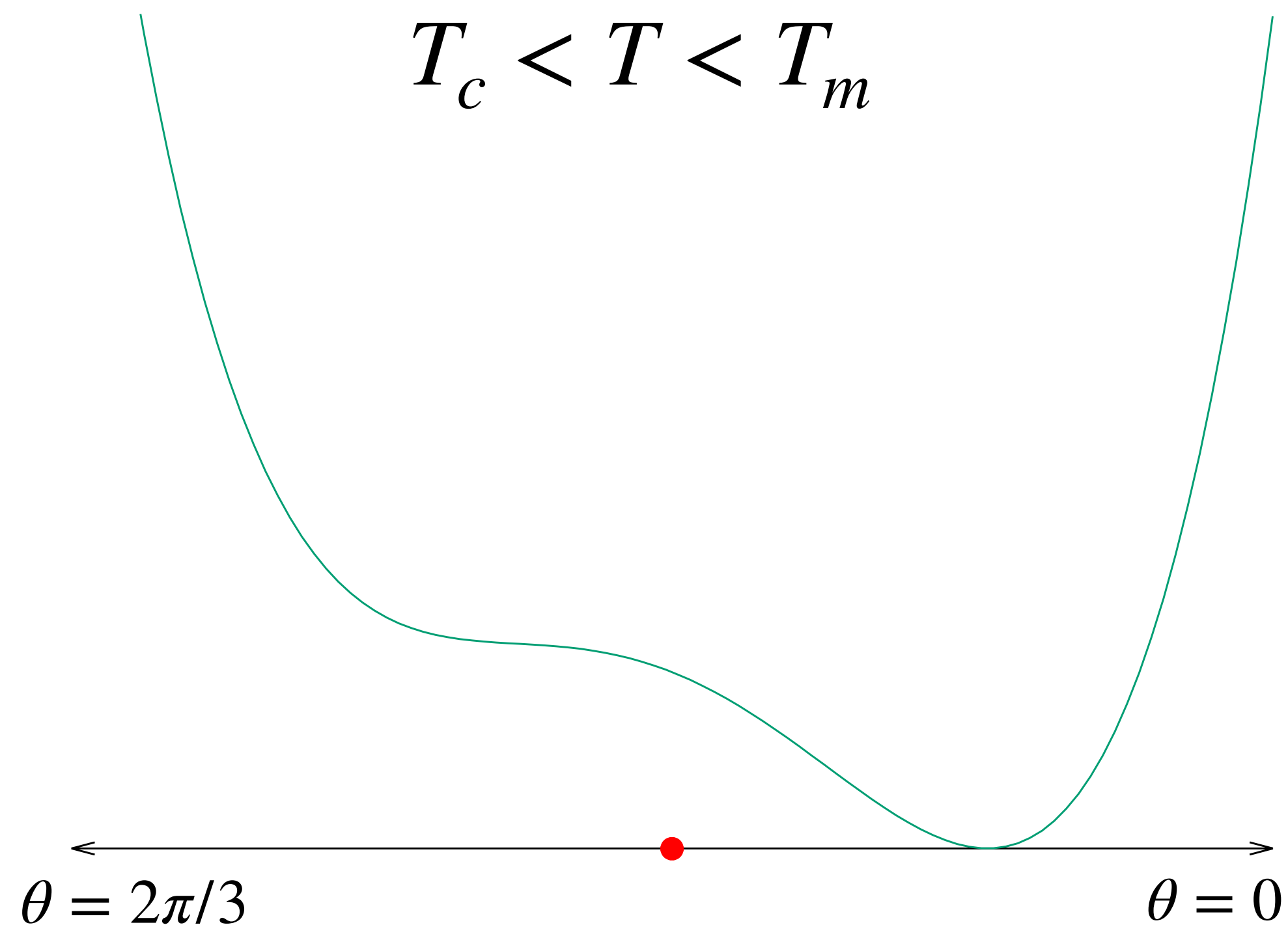
- This breaking of Z_3 symmetry leads to existence of unstable or metastable states in the deconfined phase.
- Just after phase transition, the barrier height between different vacua will be smaller, leading to unstable states for $\theta = \pm 2\pi/3$ due to dominance of explicit breaking.



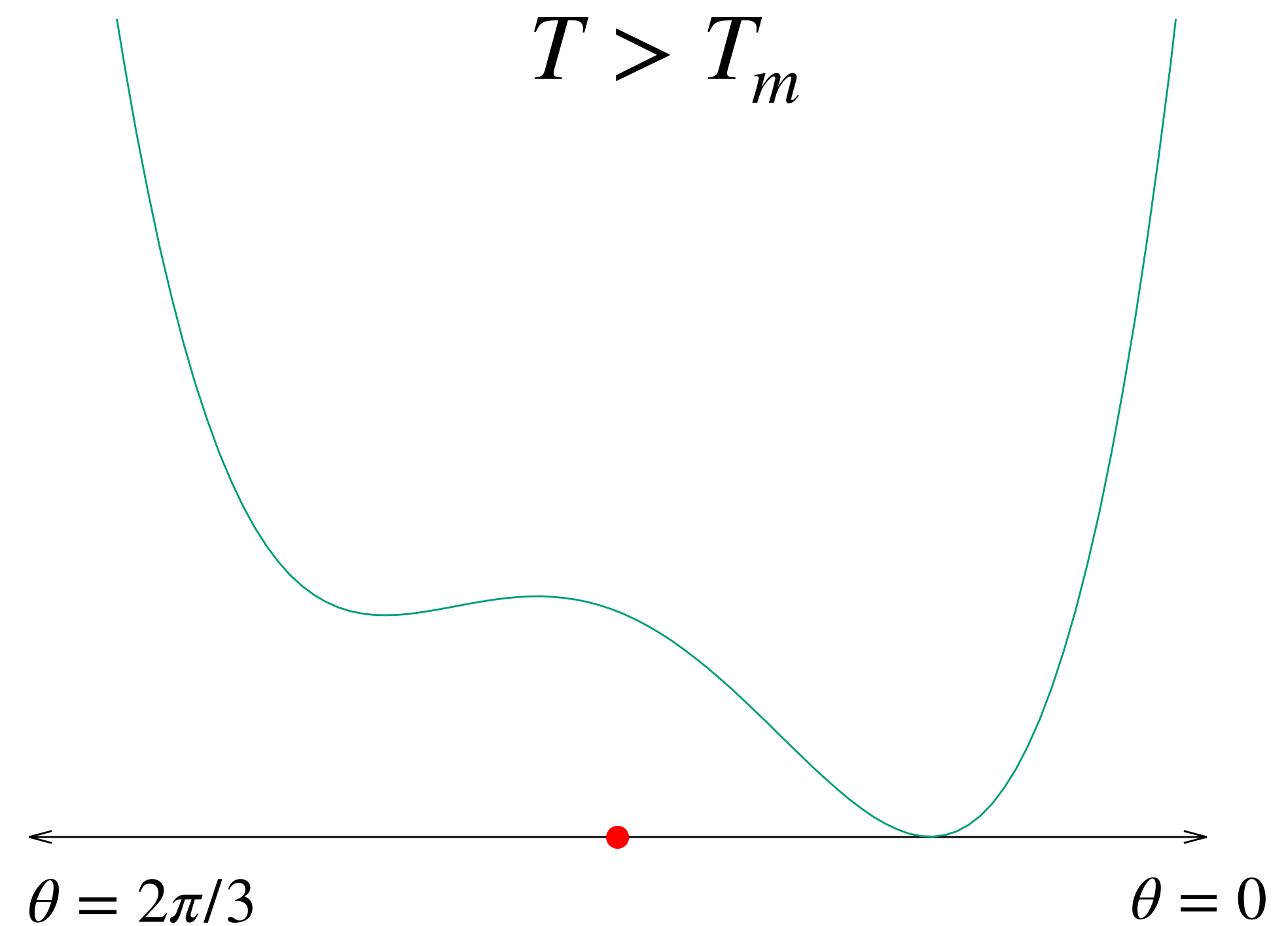
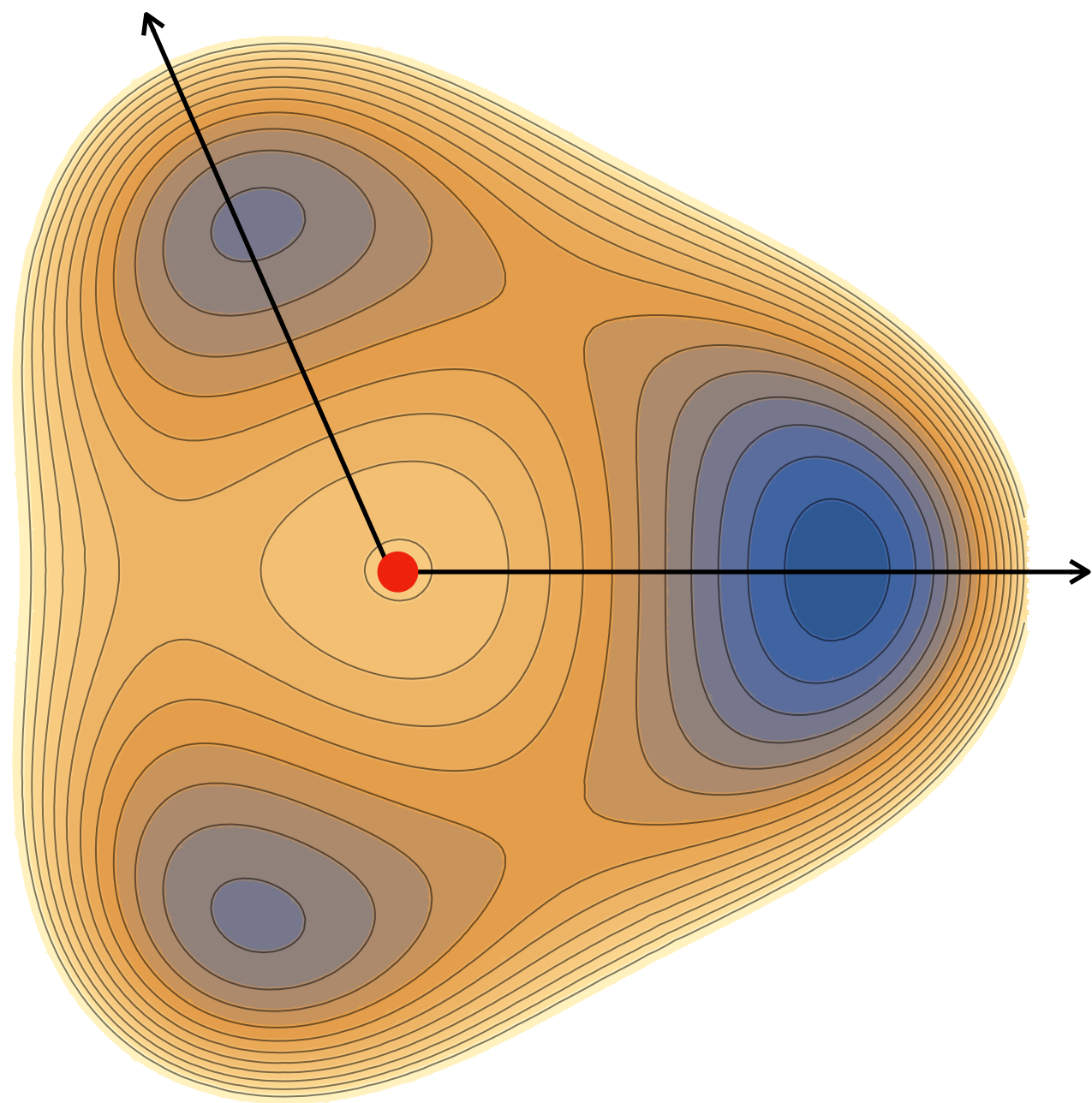
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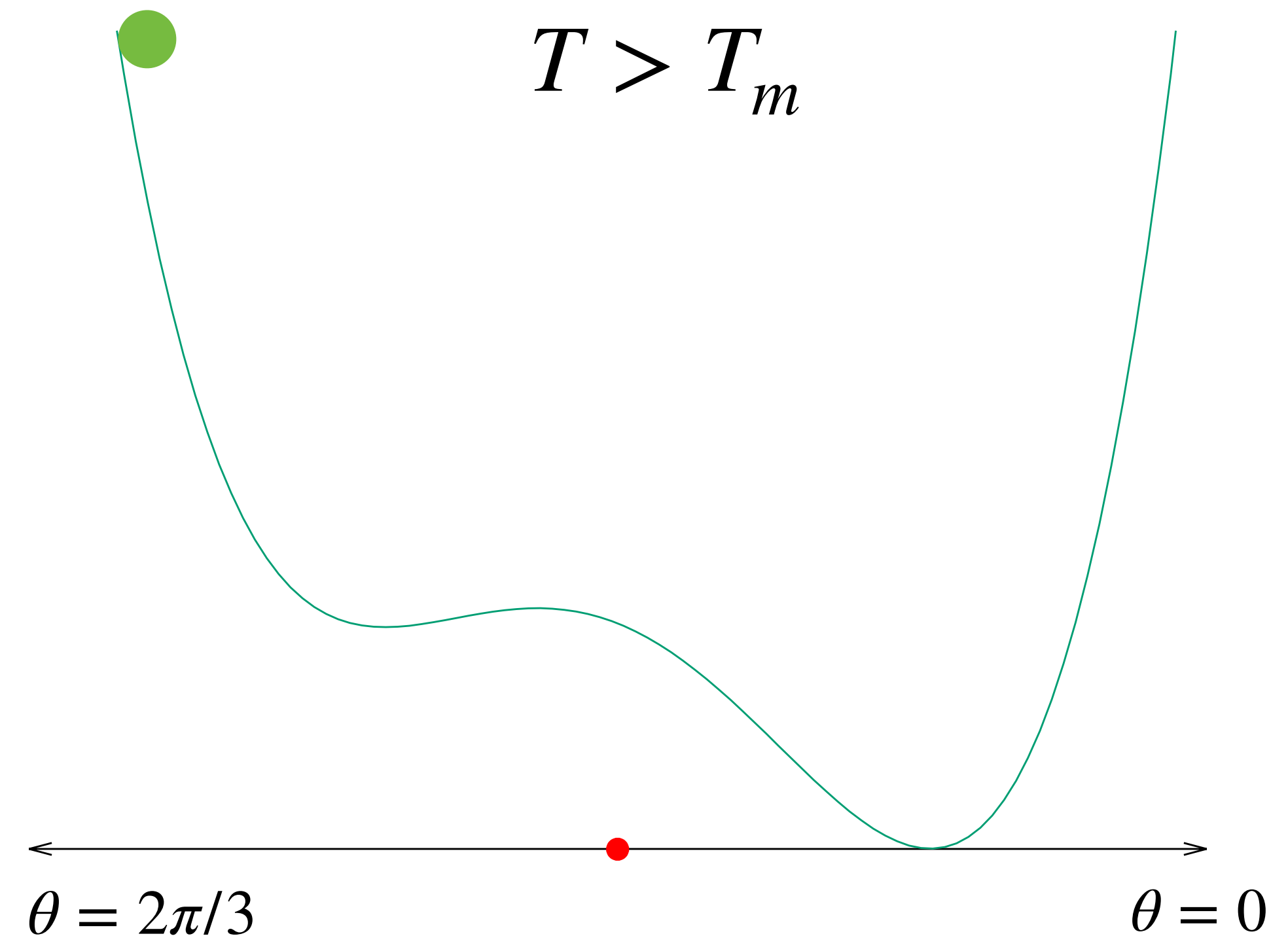
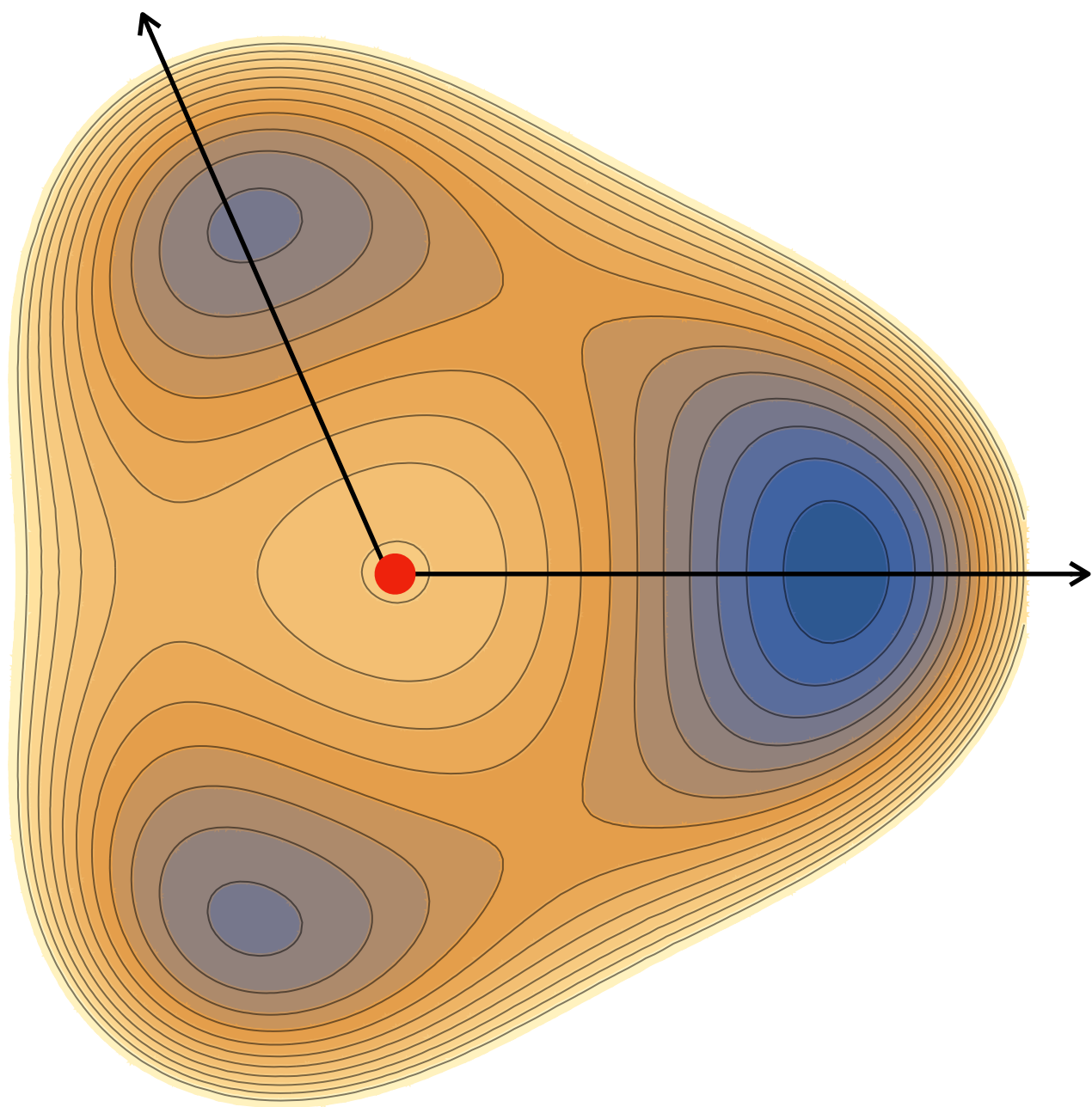
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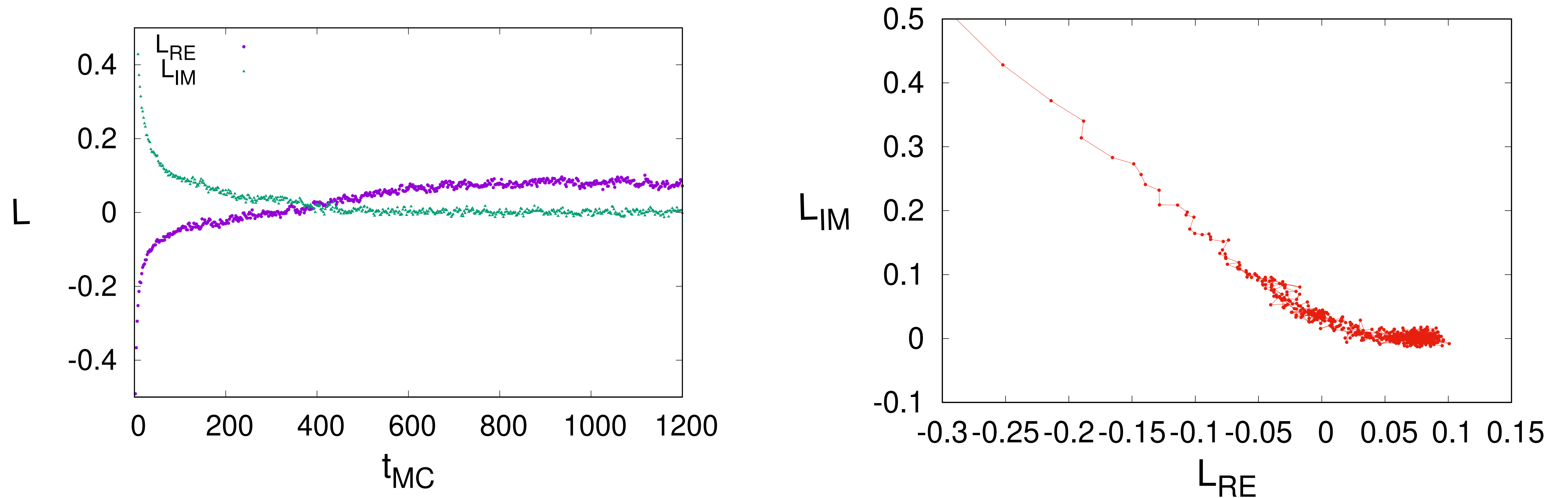
- This breaking of Z_3 symmetry leads to existence of unstable or metastable states in the deconfined phase.
- We search for the temperature at which metastable states start appearing by numerically exploring effective potential.
- As the probability for a random initial configuration to end up in the metastable state is small, we choose an initial configuration with PL having phase $\theta = \pm 2\pi/3$. This is achieved by setting $U_4(\vec{n}, n_\tau = N_\tau) = e^{\pm i2\pi/3} I$ and rest of the links are taken to be I .



- To evolve/update configurations, we take HISQ/tree action and evolve it using RHMC algorithm. MILC code is implemented for this purpose.
- Our choice of lattice action is primarily motivated by the need to use beta function results already available in literature to set the physical scale.
- Molecular dynamics along with Monte Carlo is used to evolve the configuration. Trajectory length traversed before Monte Carlo accept/reject step explores the configuration space.
- For benchmarking purpose we have reproduced finite temperature results($\langle \bar{\psi}\psi \rangle_{l,s}$, L_{bare} , etc.) of HotQCD collaborations[#] Phys. Rev. D 90, 094503 (2014).
- So, bare quark masses are such that $m_l = m_s/20$ and resulting pion masses are around $160MeV$.

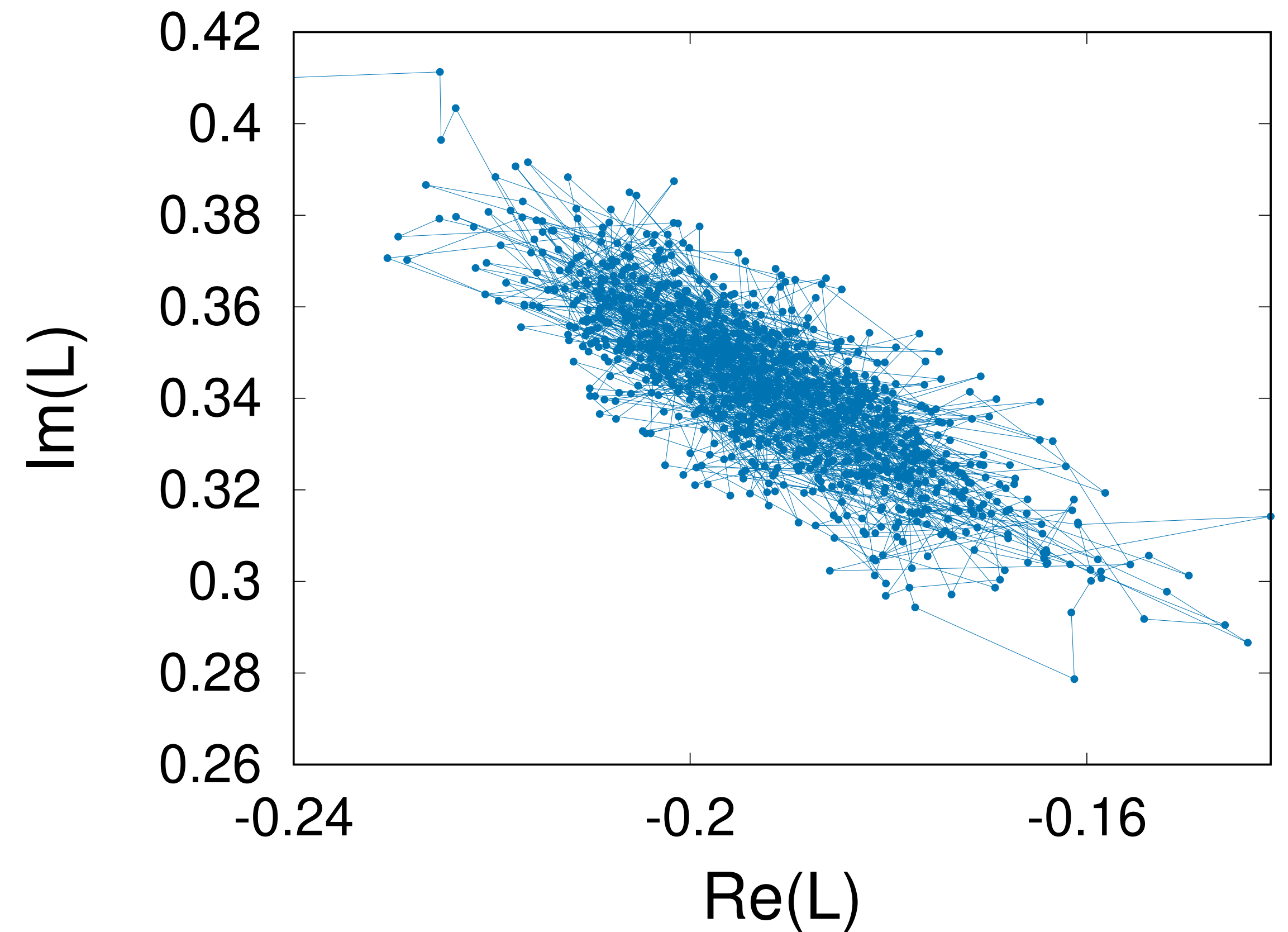
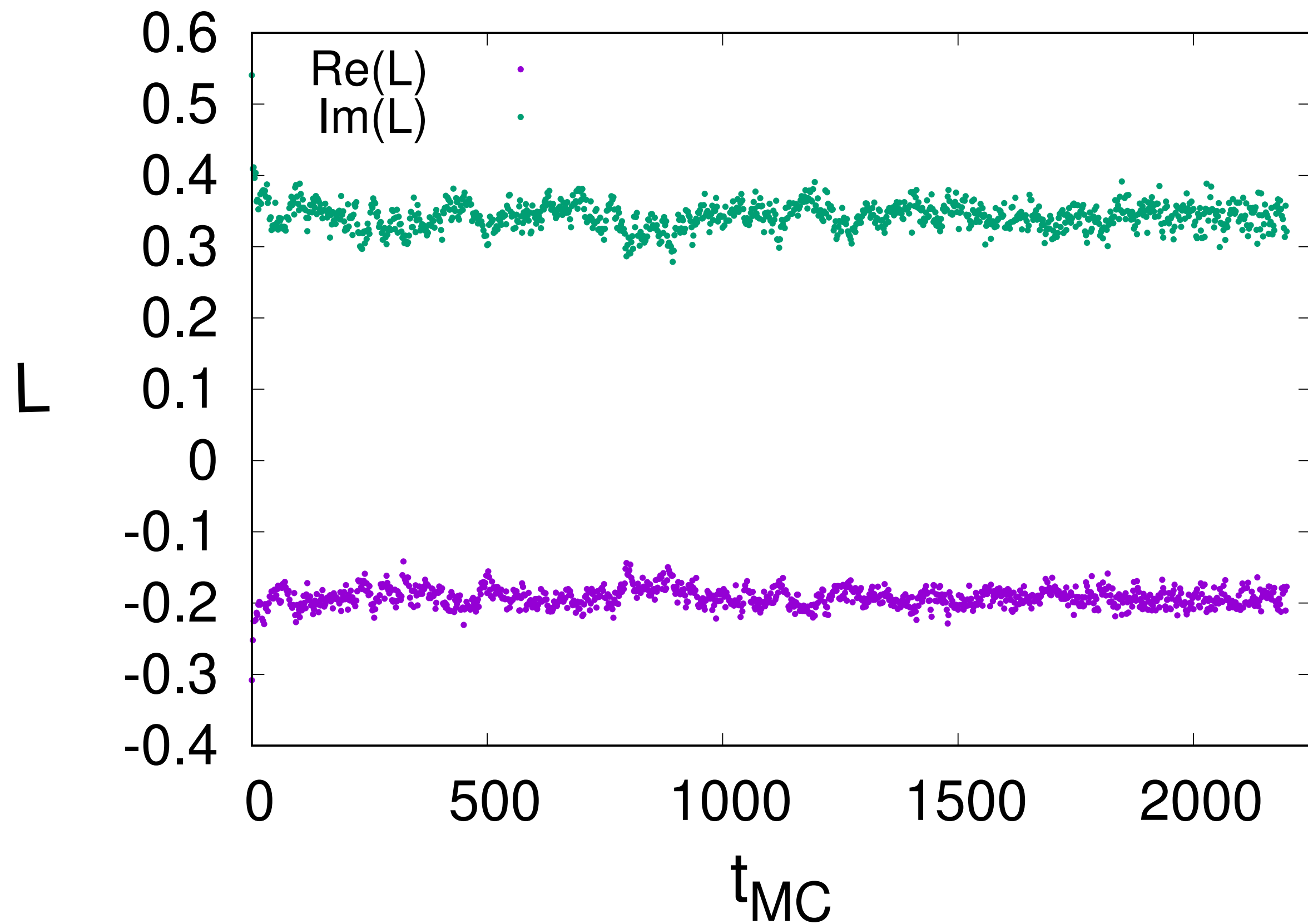
[#]A. Bazavov et al. [HotQCD], Equation of state in (2+1)-flavor QCD, Phys. Rev. D 90, 094503 (2014)

Results

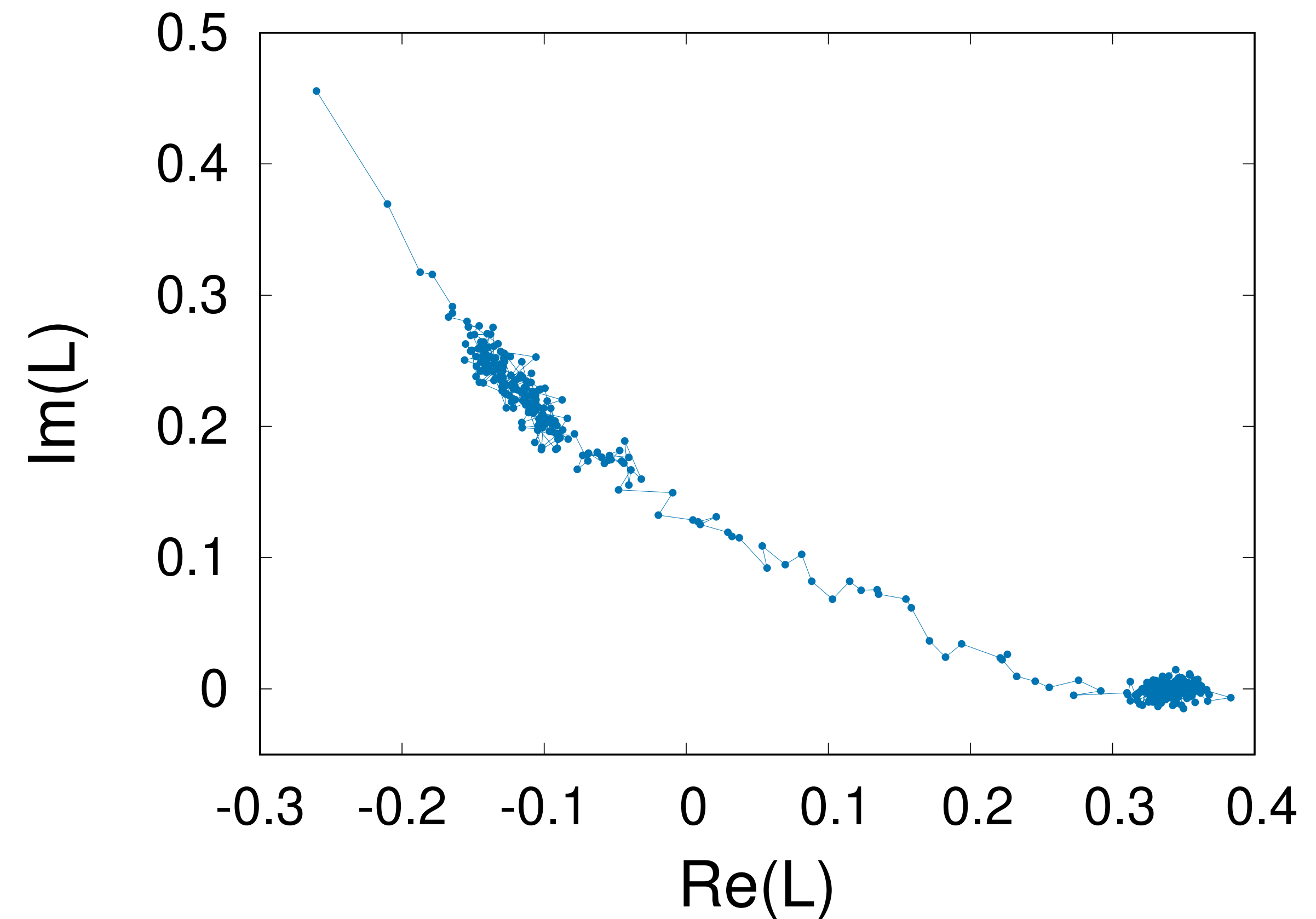
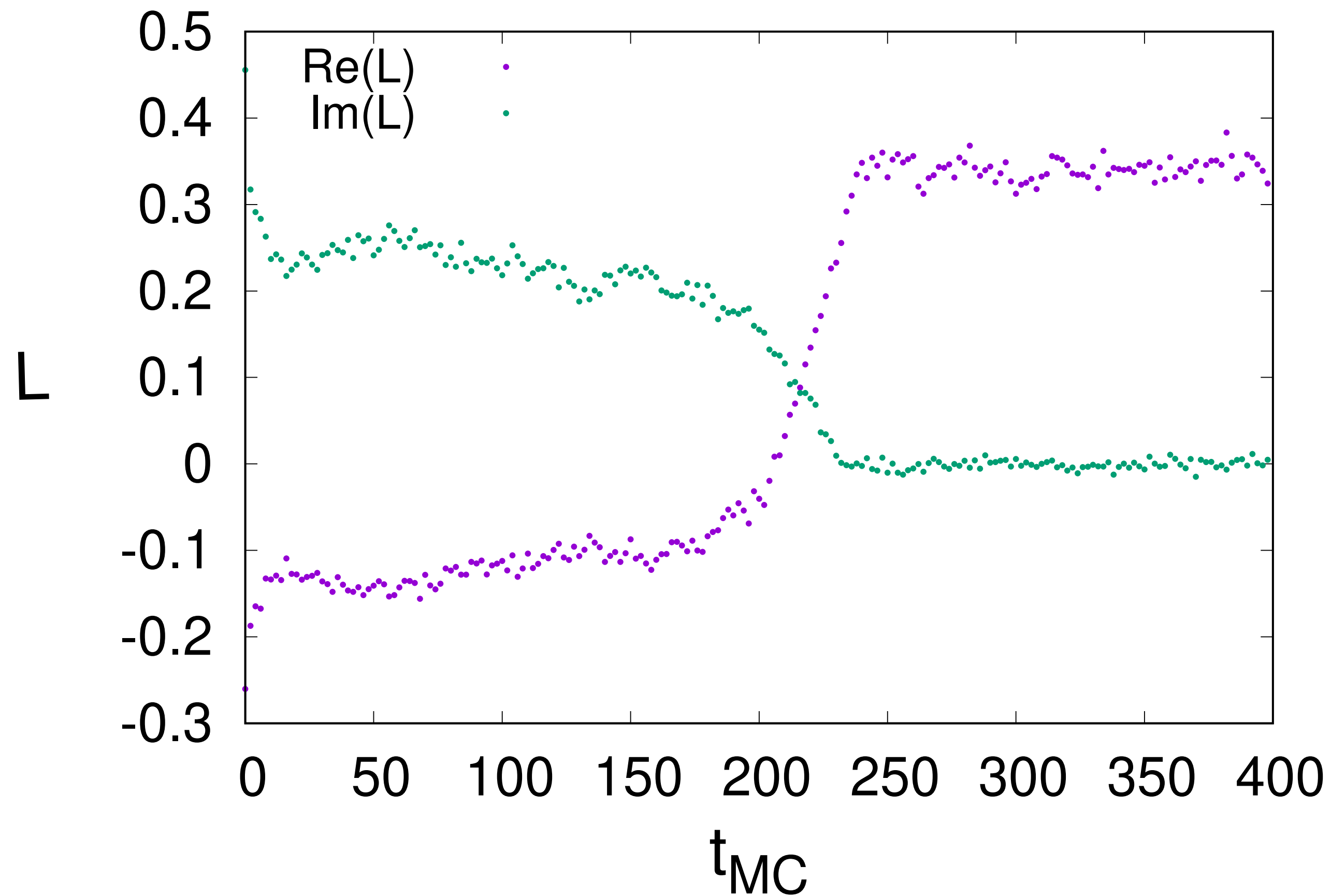


- For temperature ≤ 370 MeV, no signature of metastable region was observed.
- For $T = 205$ MeV, the evolution shows thermalisation above $t_{MC} \sim 900$.

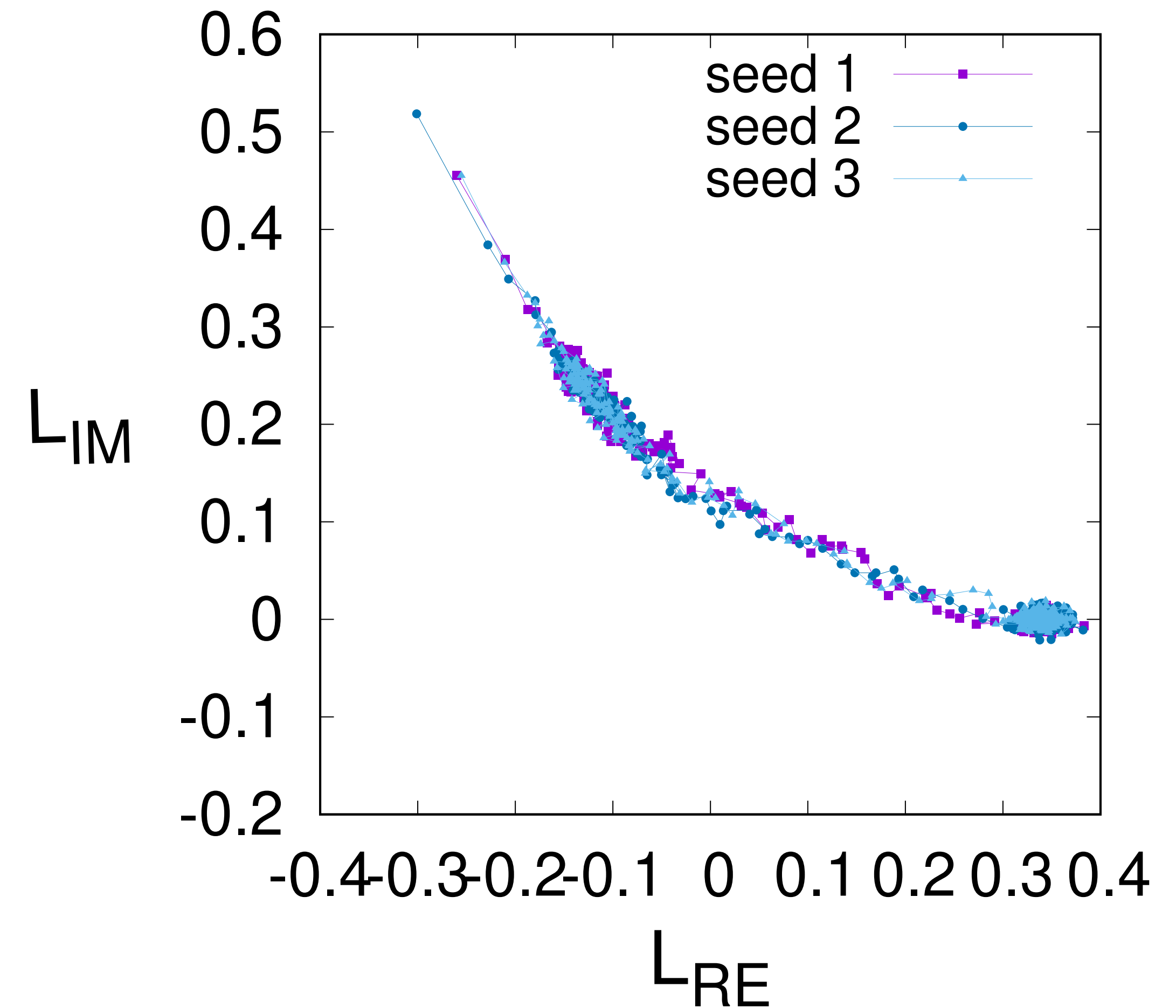
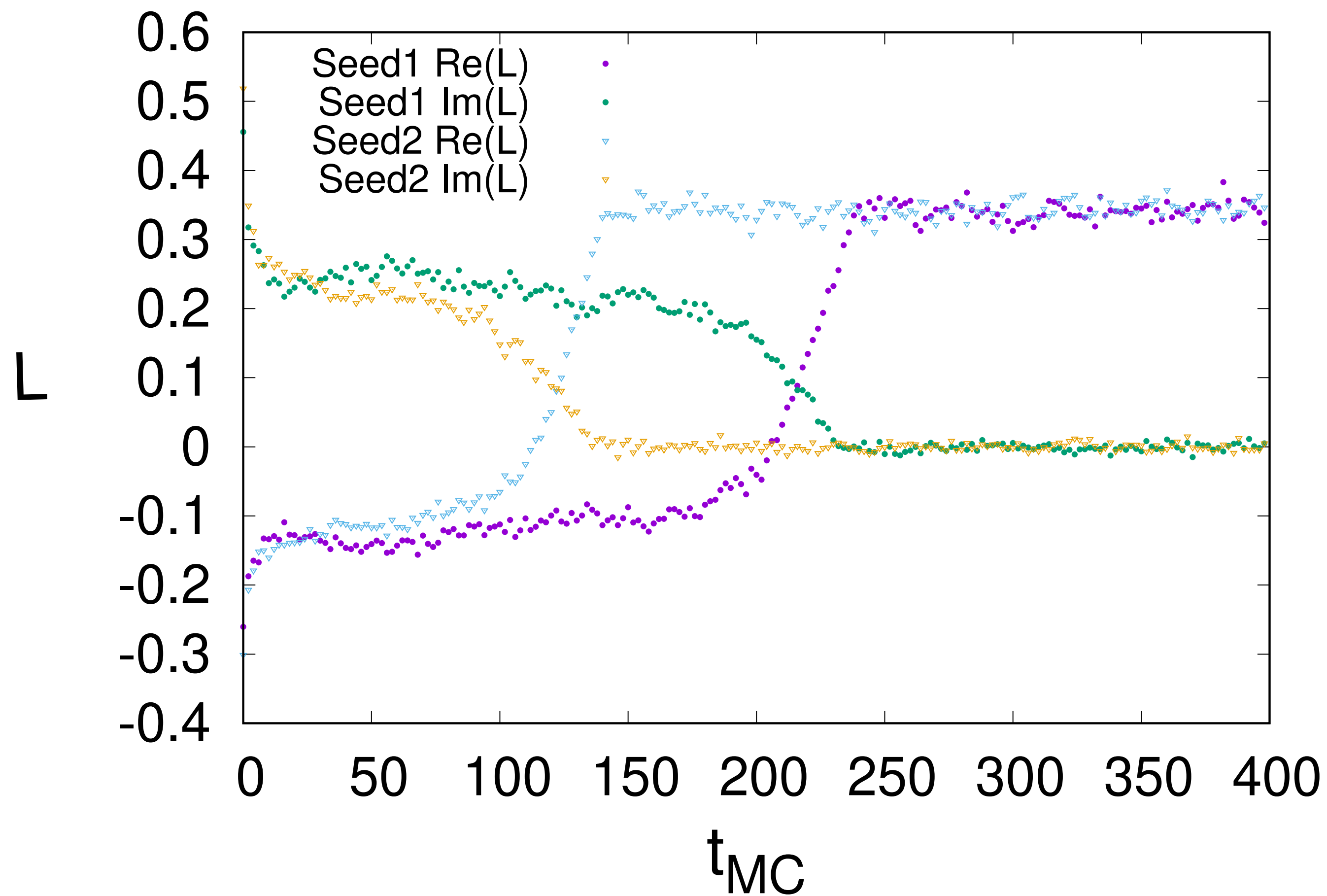
- For the highest temperature(we considered) of $T = 815MeV$, the metastable state did not decay for observed simulation time.
- Different step sizes were considered in evolving this to consider effect of fluctuations on metastability.



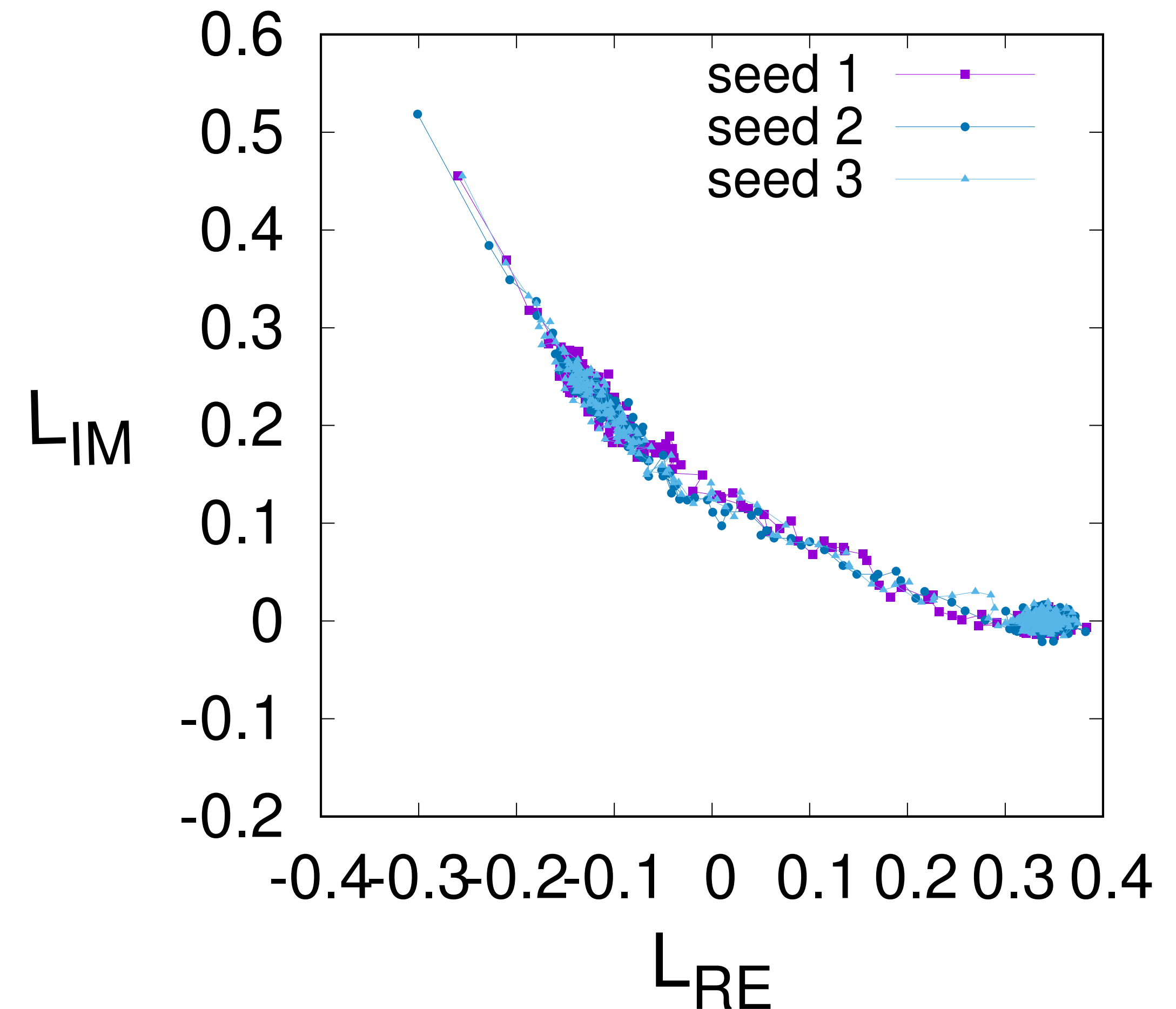
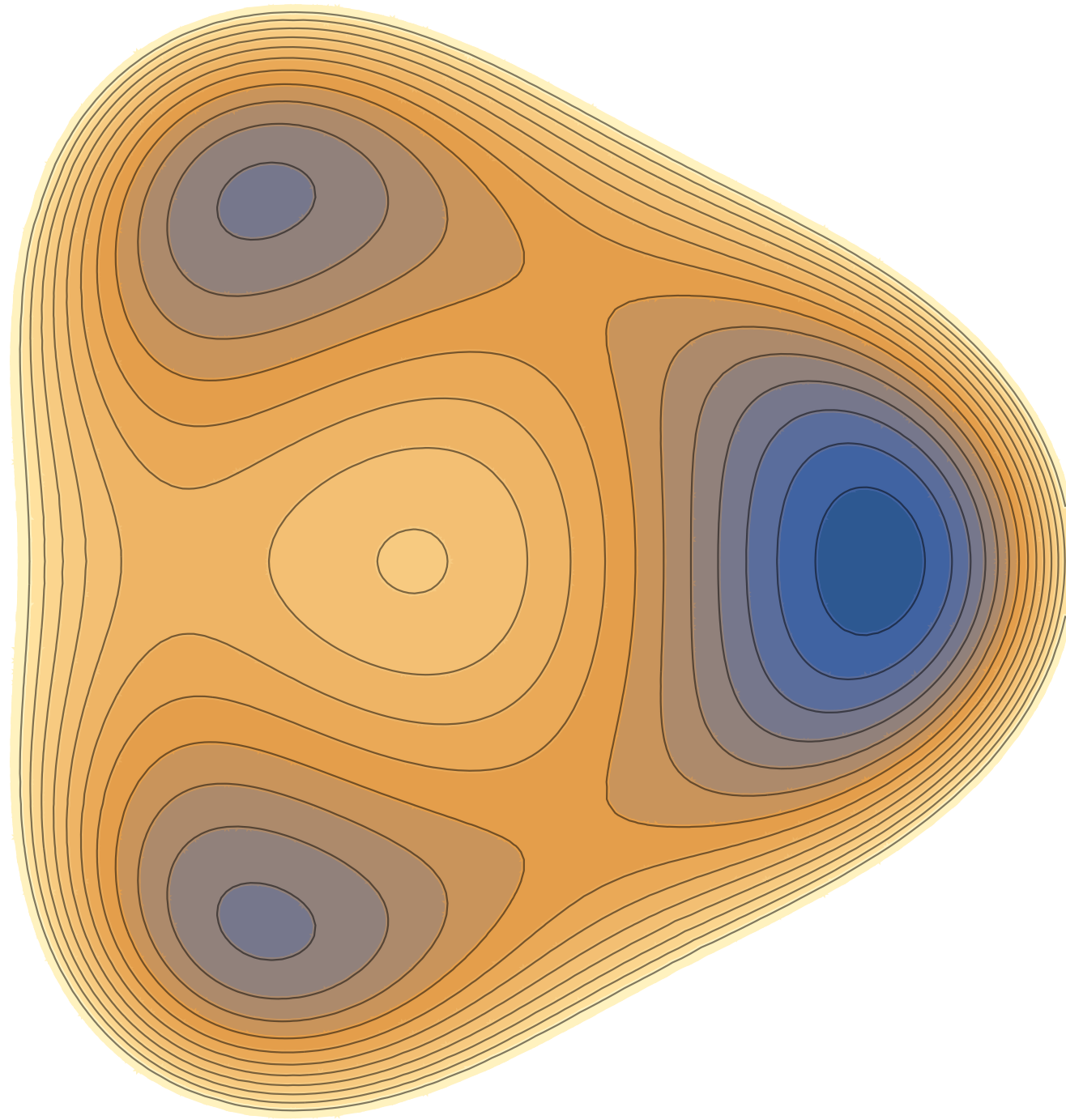
- These Metastable states will eventually decay due to fluctuations. For temperature $T = 546\text{MeV}$ we observe such a decay.



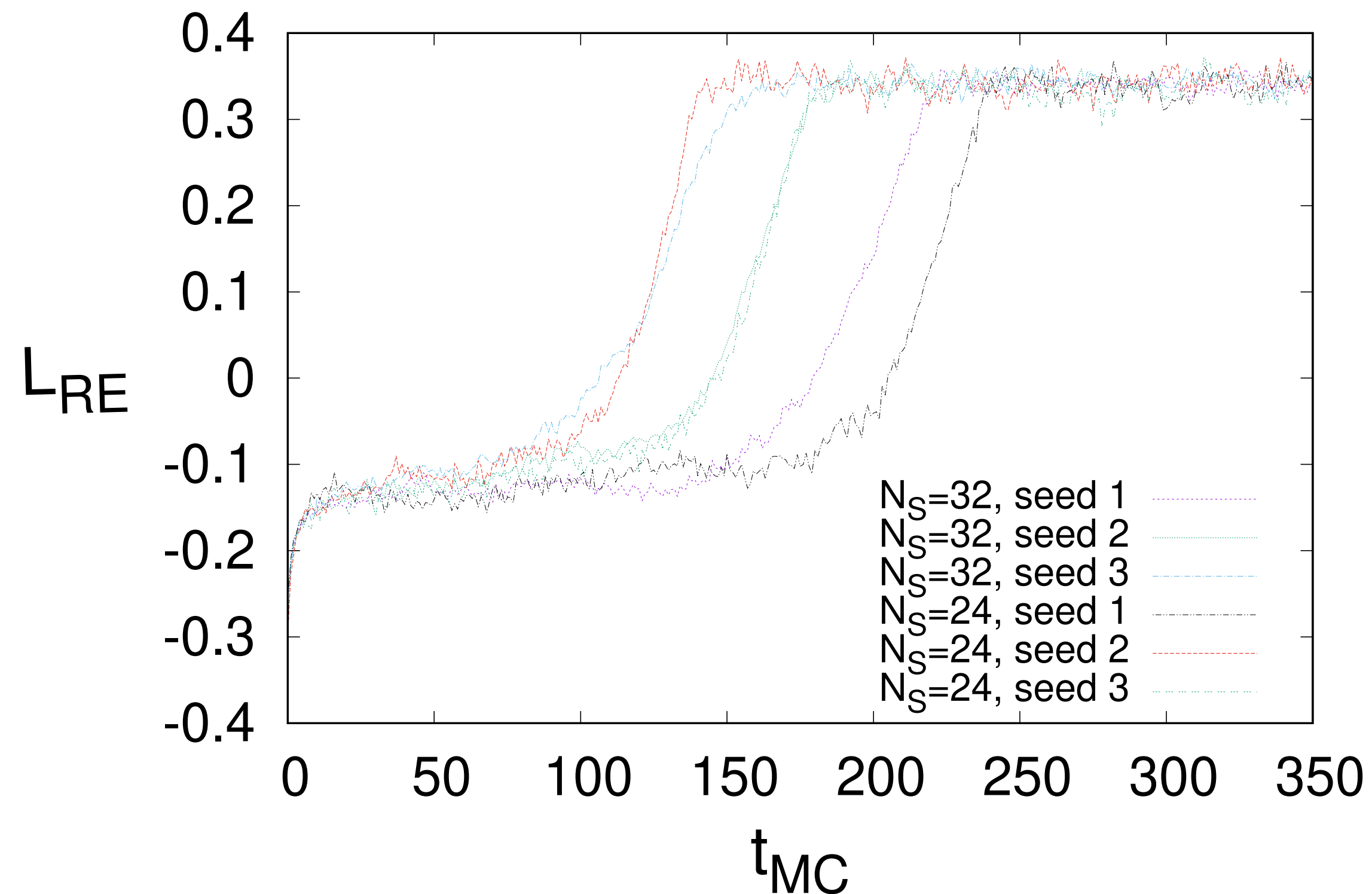
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- To check these are not once occurrence event, we evolve same initial configuration via different trajectories.

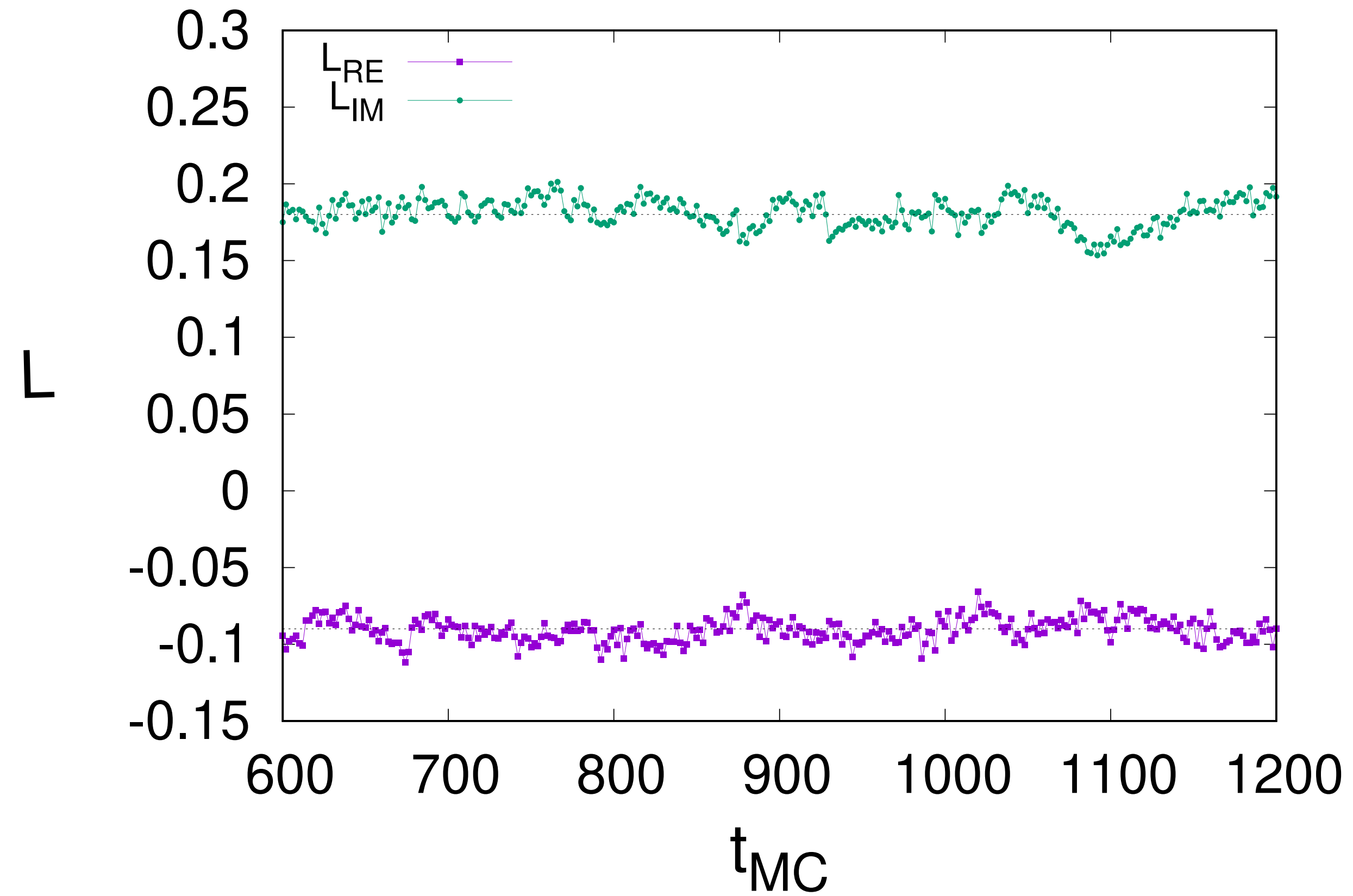


- These Metastable states will eventually decay due to fluctuations. For temperature $T = 546 MeV$ we observe such a decay.
- Effective potential gives some idea of why the trajectory for decay follows a particular path.



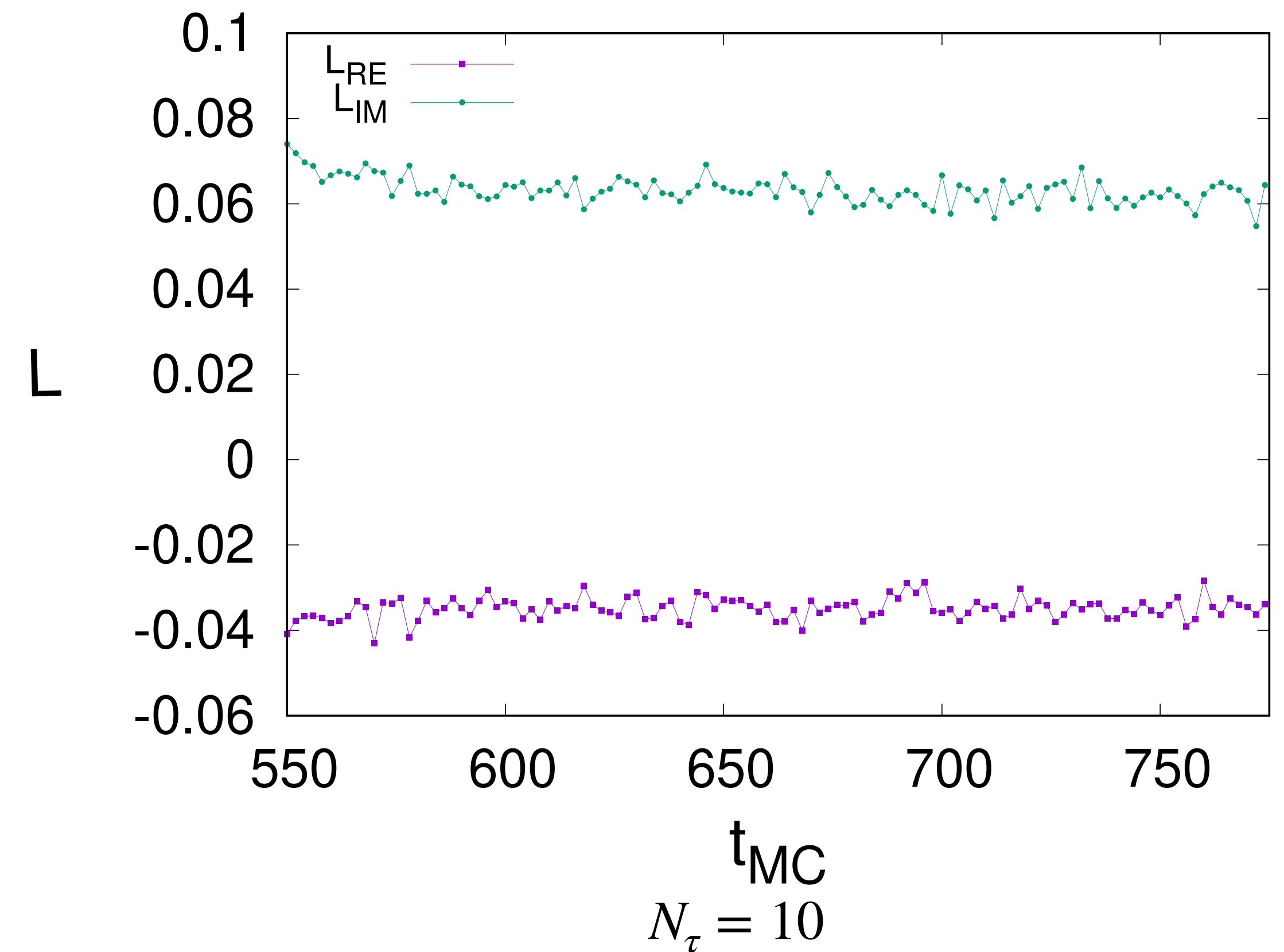
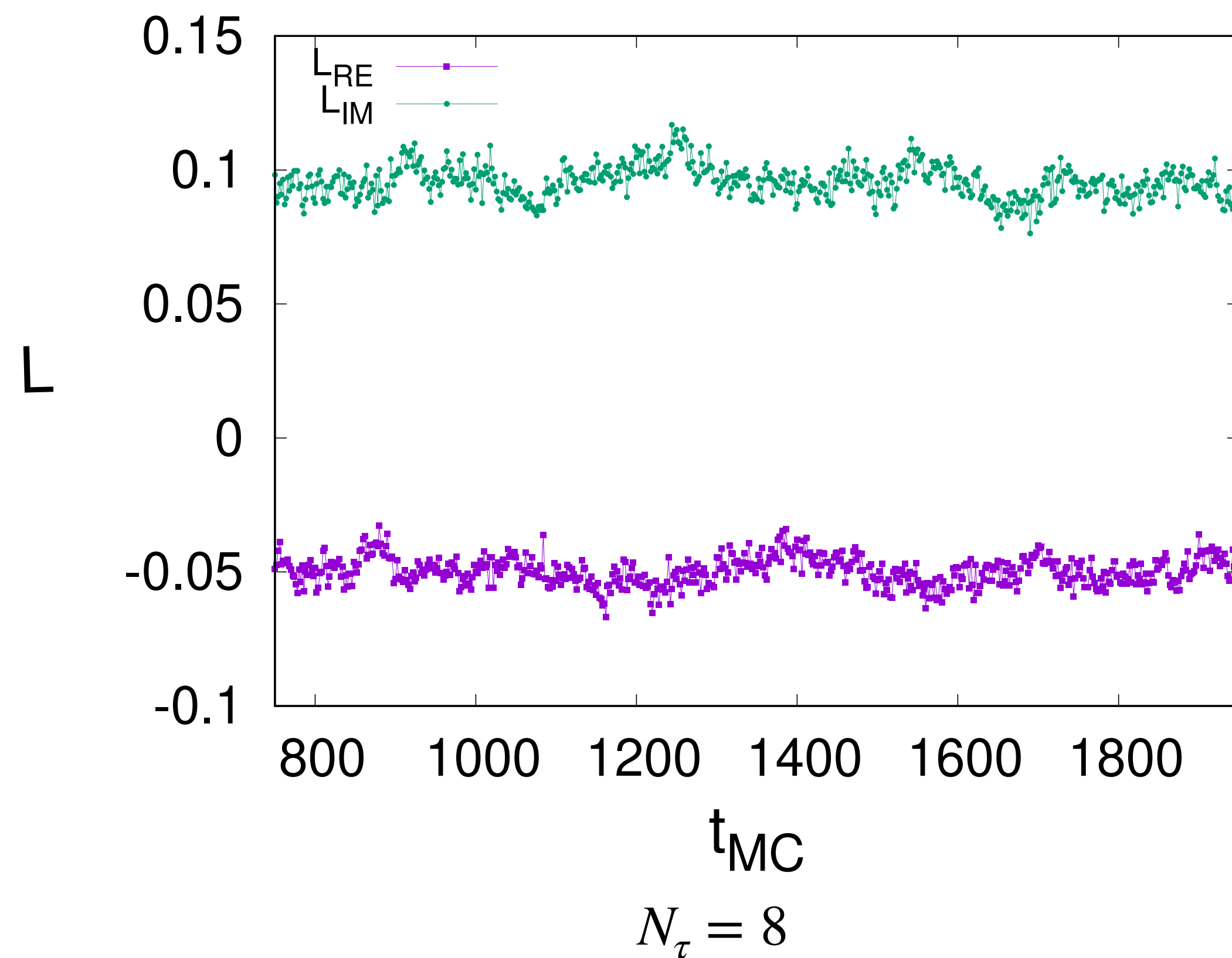
- We have also studied finite size effects on metastable region on determination of T_m .
- The evolution of real part of Polyakov loop for two volumes and using different random seeds shows no qualitative difference.





- For the lowest temperature of $T = 446$ MeV, we observe a clear signature of metastable state.
- Hence, we estimate $370 \text{ MeV} \leq T_m \leq 446 \text{ MeV}$.

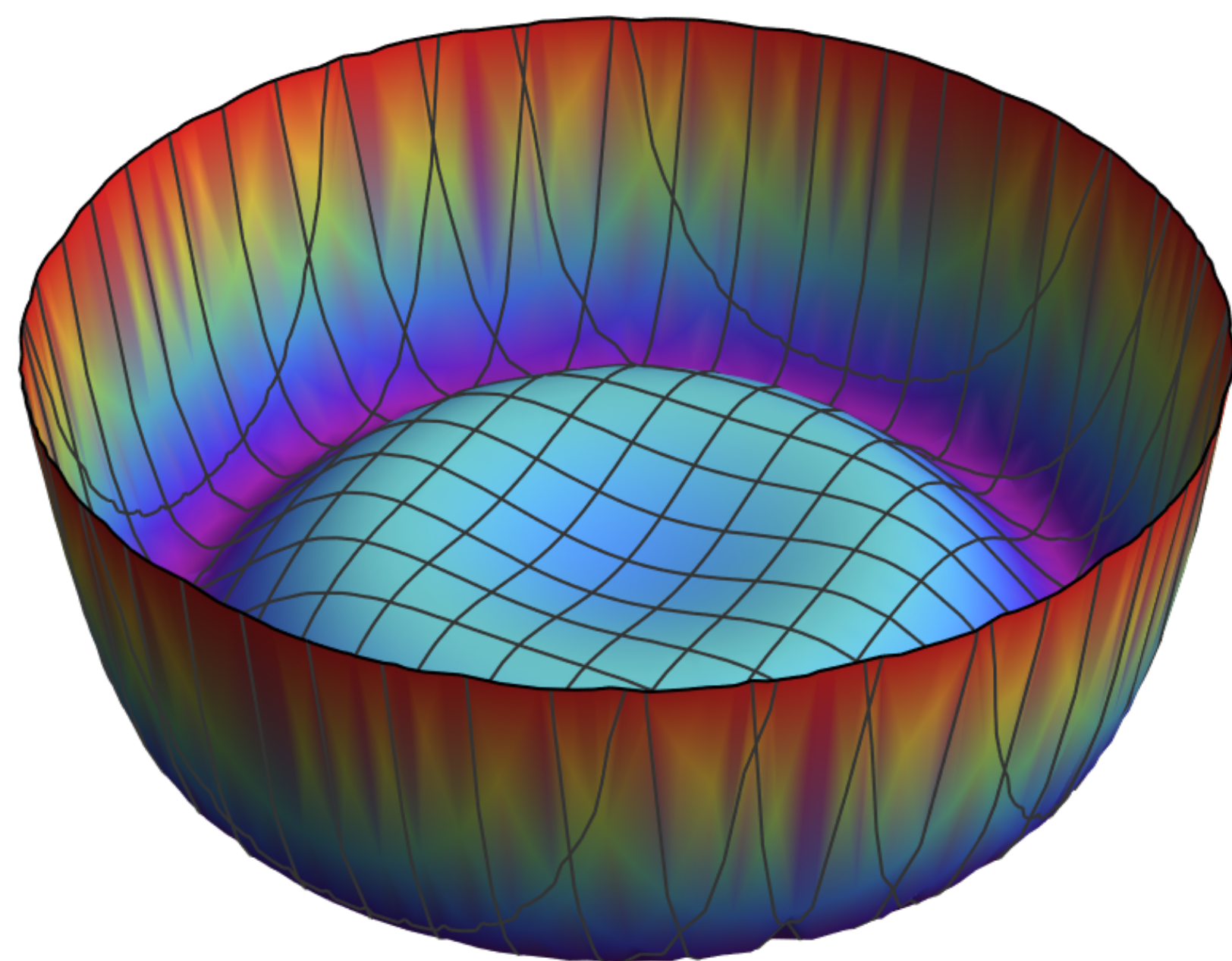
- For $T = 446$ MeV, we have studied cutoff effects. These effects reduce with increase in N_τ .
- With increase in N_τ from 6 to 10, we continue to observe the metastable states at this temperature.



Summary

- Our current estimate of T_m is $370MeV < T_m \leq 446MeV$.
- Currently, we are studying lattice cutoff effects on determination of T_m .
- Bubbles of Metastable states may occur in the background of stable vacuum, during heavy ion collisions.
- The presence of such bubbles as domains may affect QGP.

Thank You!

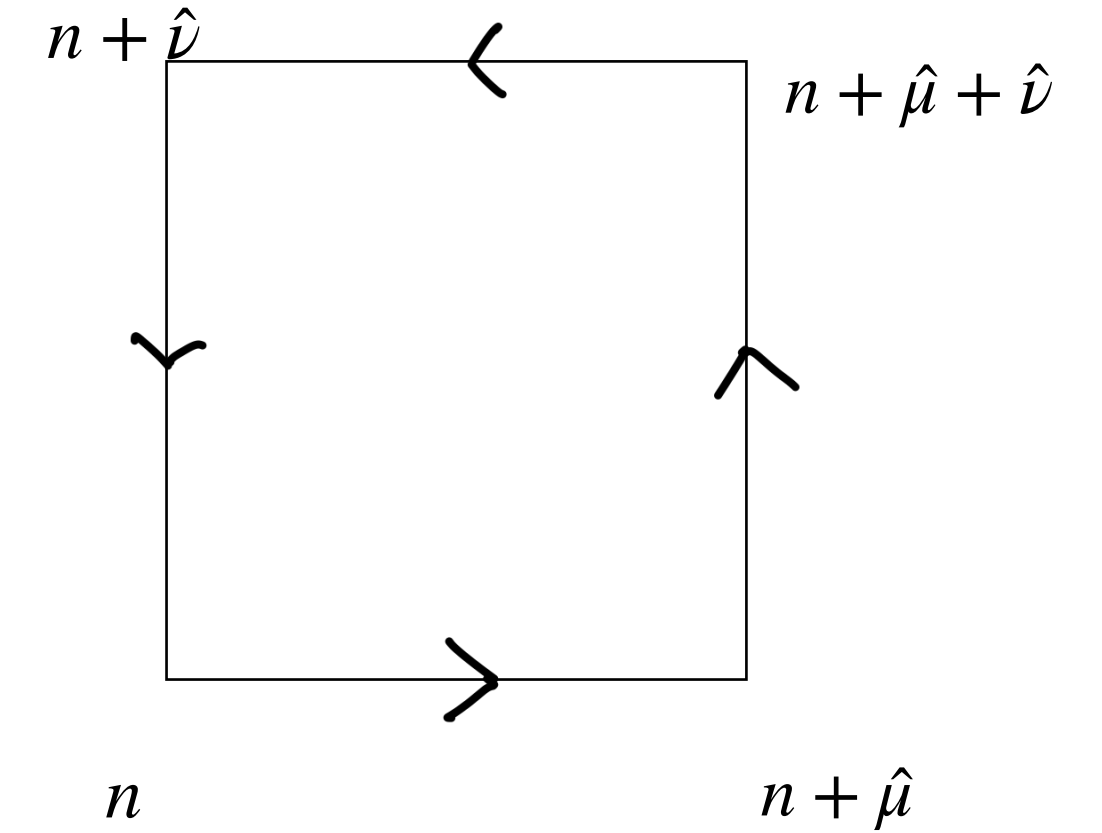


- The lattice action

$$S = S_G + S_F$$

$$S_G = \beta \left(C_P \sum_P \left(1 - \frac{1}{3} \text{ReTr}(P) \right) + C_R \sum_R \left(1 - \frac{1}{3} \text{ReTr}(R) \right) \right)$$

$$n \equiv (n_1, n_2, n_3, n_4) \quad P \equiv U_\mu(n) U_\nu(n + \hat{\mu}) U_\mu^\dagger(n + \hat{\nu}) U_\nu^\dagger(n)$$



- Fermionic action(Highly Improved Staggered Quarks) is such that contribution to the partition function is given by $\prod_f \det \left(\mathcal{M}_f \right)^{1/4}$.
- Grassmann variables can not be directly put on a computer, hence one uses pseudo fermion fields, ϕ_f

$$\det[\mathcal{M}_l \mathcal{M}_l^\dagger]^2 \det[\mathcal{M}_s \mathcal{M}_s^\dagger] \propto \int \mathcal{D}[\phi_l] \mathcal{D}[\phi_s] e^{-\phi_l^\dagger (\mathcal{M}_l \mathcal{M}_l^\dagger)^{-2} \phi_l - \phi_s^\dagger (\mathcal{M}_s \mathcal{M}_s^\dagger)^{-1} \phi_s}$$