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Relaxation dynamics and the free energy near the phase boundary of the 3D kinetic Ising model

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Reference:

[1] Ranran Guo, Xiaobing Li, Yuming Zhong, Mingmei Xu, Jinghua Fu, and Yuanfang W, arXiv:2412.18909v2

Outline

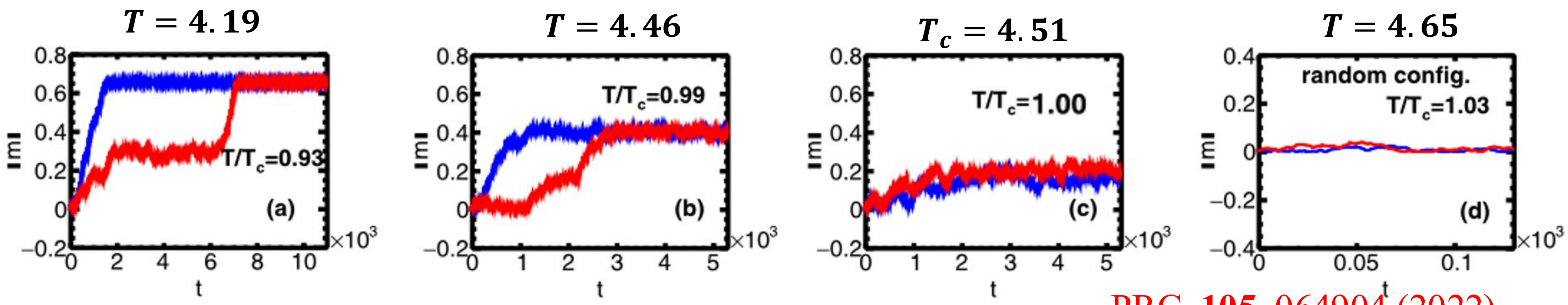
- Motivation
- Ising Model
- Characteristics of the free energy landscape
  - near the (Critical Point)CP
  - near the 1st order Phase Transition Line (1st-PTL)
- Relative variance of the equilibration time and non-self-averaging
- Summary

Motivation

The relaxation dynamics near phase boundaries is a fundamental problem in non-equilibrium statistical physics.

■ Well-established: critical slowing down.

■ Poorly understood: how systems relax at the first-order phase transitions (1st-PT).



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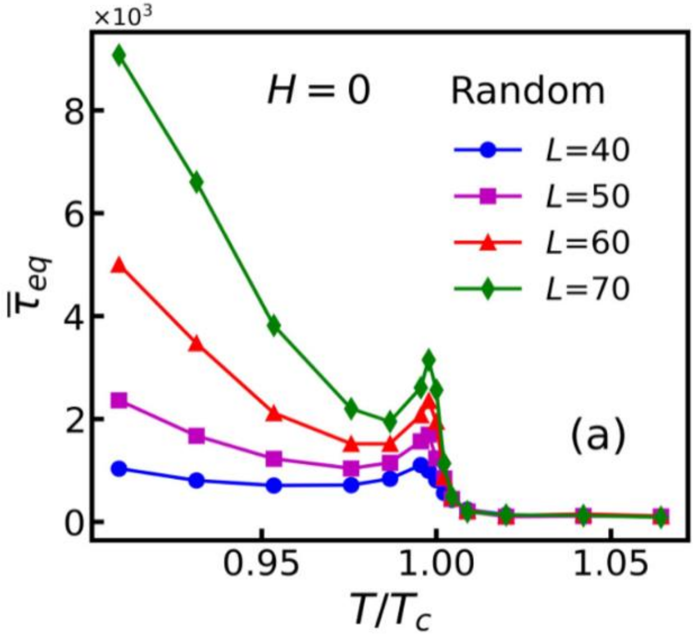
➢ It is found that the nonequilibrium evolution at $T > T_c$ lasts very shortly, and the influence is much weaker than that at $T < T_c$.

Motivation

PRE. 111, 064115 (2025)



$$\bar{\tau}_{\mathrm{eq}} = \frac{1}{\mathcal{N}} \sum_{j=1}^{\mathcal{N}} \tau_{\mathrm{eq}}^{j}$$

τ_{eq} is defined by the number of sweeps required for the order parameter to reach the steady value.
N is the number of evolution processes.

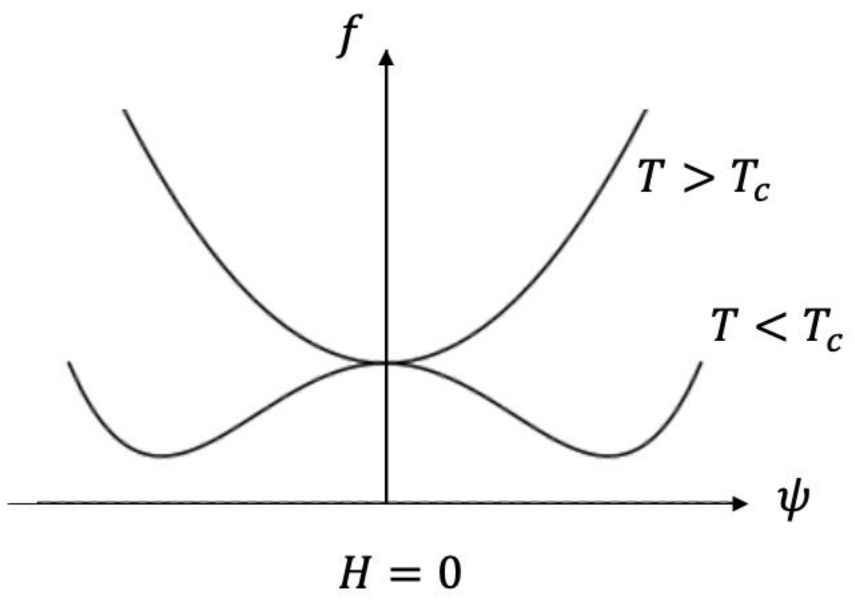
- The average equilibration time $\bar{\tau}_{eq}$ along the 1st-PT line exhibits an ultra-slow relaxation, which is caused by the complex structure of the free energy.

Research status

- **Pseudo-critical slowing down** – the relaxation time diverges near the spinodal point due to the vanishing second derivative of free energy.
- **Exponential slowing down** – the tunneling time between coexisting phases grows exponentially with system size, governed by the free energy barrier.
- **Metastable lifetime** – shows a similar exponential dependence on system size due to the free energy barrier.

The dynamical slowing down observed across different timescales can be attributed to the structure of the underlying free energy landscape.

Research status



- What would be the free energy landscape near the first-order phase boundary far below T_c?

- Would it resemble the behavior near T_c?

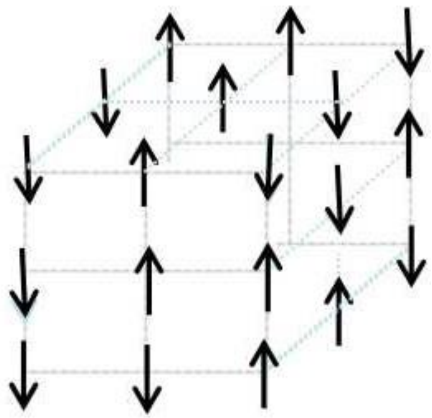
Ising Model

Metropolis algorithm

Constant nearest-neighbor interactions J

Uniform external field H

$$E_{\{s_i\}} = -J\sum_{\langle ij\rangle} s_i s_j - H\sum_{i=1}^{N} s_i$$



$N = L^3$

$s_i = +1, -1$

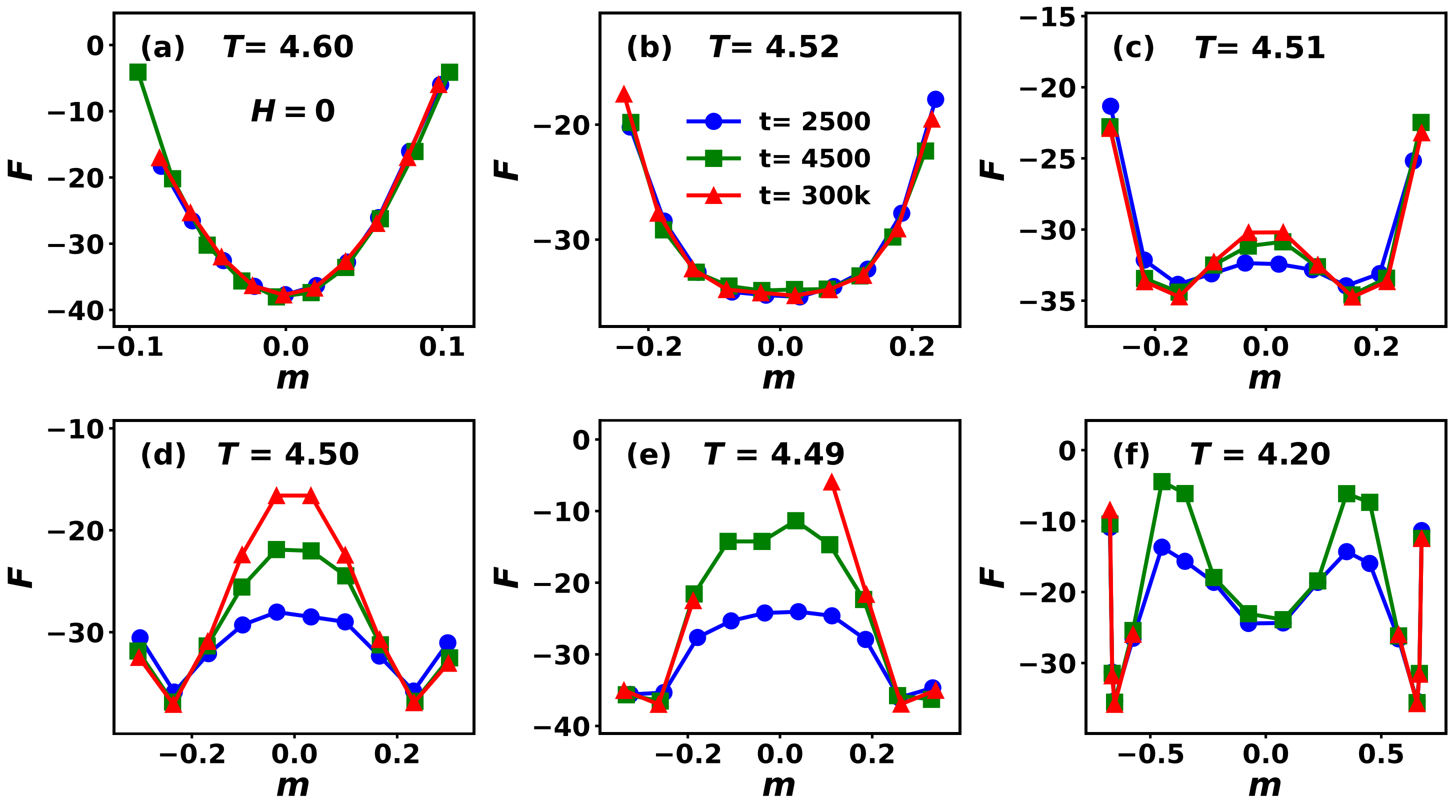
Partition function

$$Z(T,H) = \sum_{\{s_i\}} \exp(-E_{\{s_i\}}/k_B T)$$

The restricted free energy :

$$F(m) = -k_B T ln Z = -k_B T ln \sum_{k} \delta(m_k - m)\exp(-E_k/k_B T)$$

The free energy landscape along the phase boundary

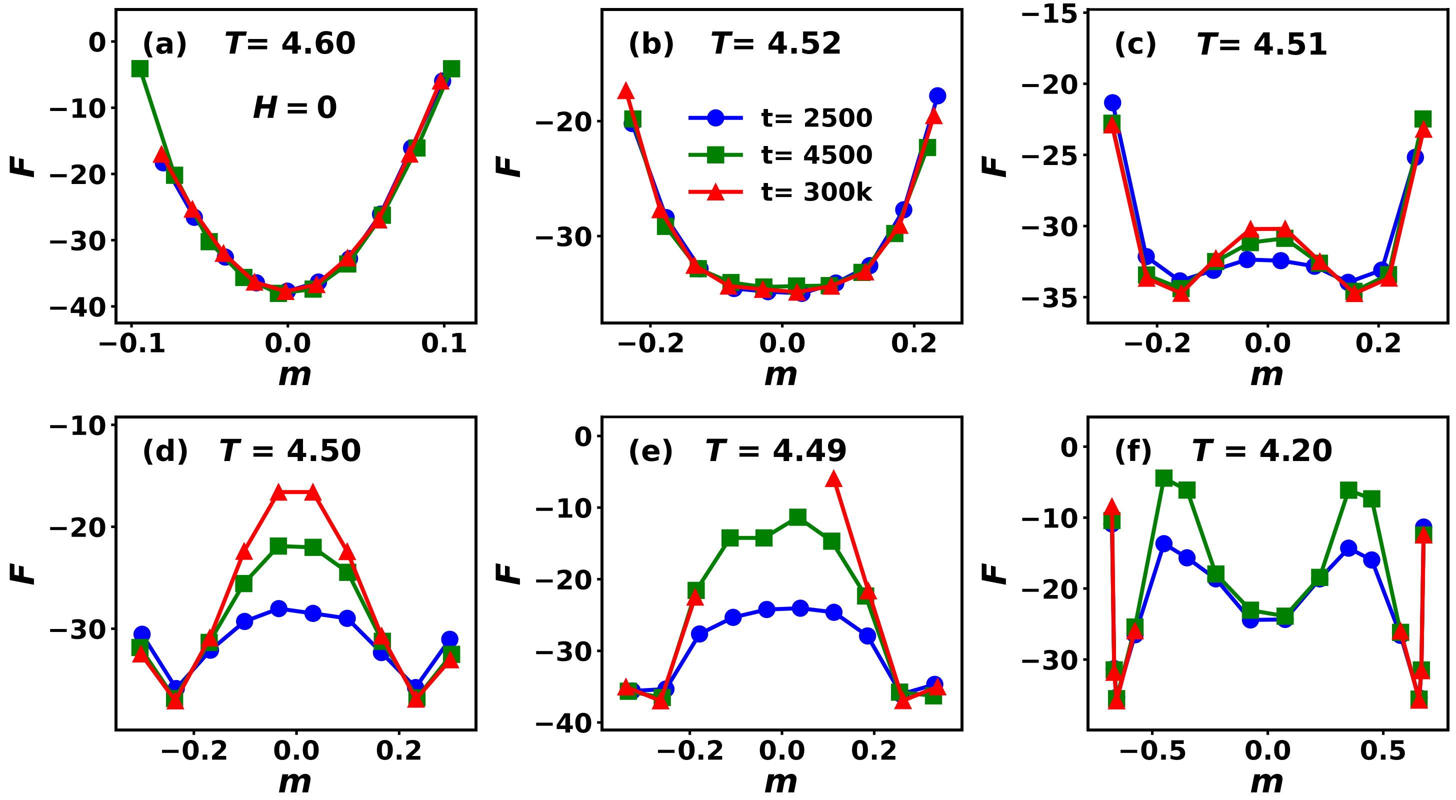


t=2500: only a fraction of systems reach equilibrium
t=4500: equilibrium fraction increases
t=300k: almost all systems reach equilibrium

- Near the critical point, the double-well of the free energy agrees with the Landau-Ginzburg–theory.

- Far below T_c, pre-equilibrium free energy forms a barrier–well–barrier structure, trapping the system at m = 0.

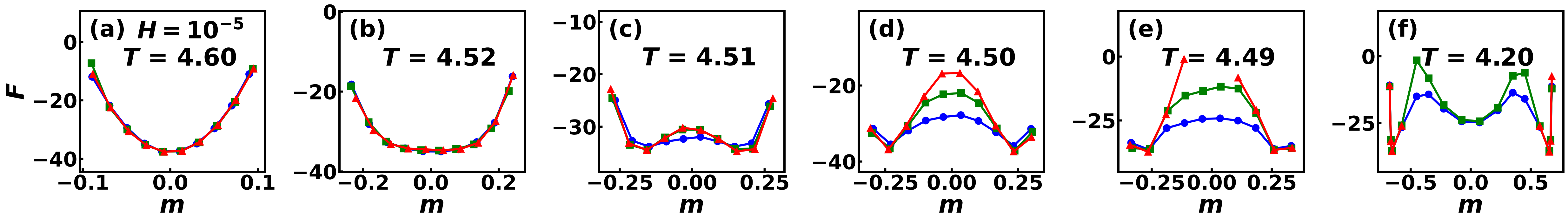
The free energy landscape along the phase boundary



- Near the critical point, the double-well of the free energy agrees with the Landau-Ginzburg–theory.

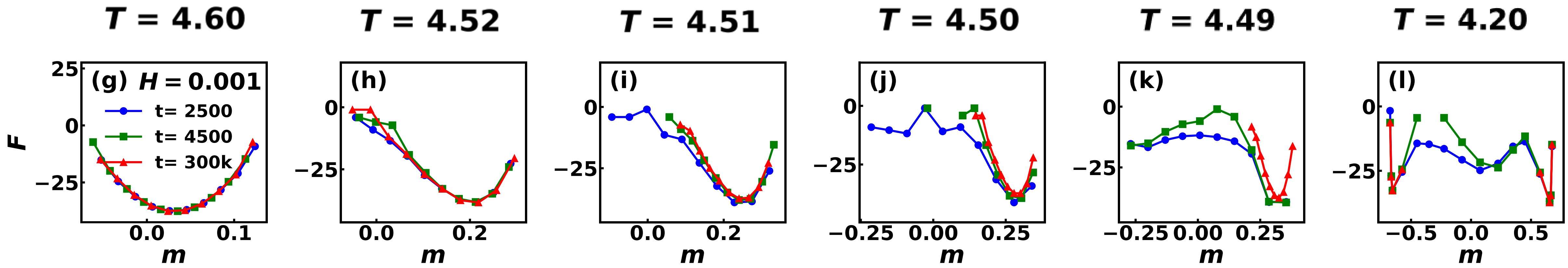
- Far below T_c , the growing barrier results the ultra-slow relaxation.

The free energy landscape near the phase boundary



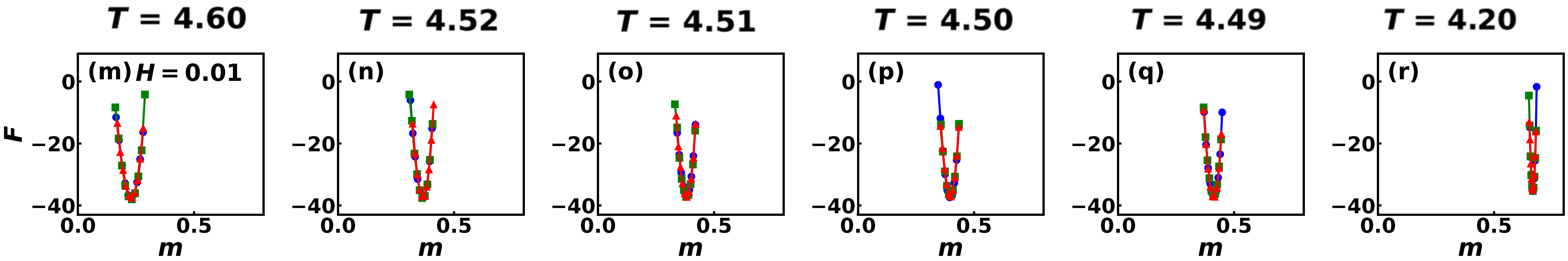
- ➢H=0.00001: F (m) maintains identical landscape to the zero-field case across all temperatures.

The free energy landscape near the phase boundary



➢H=0.001: the symmetric profile becomes asymmetric, with the minimum shifting rightward along the magnetization axis.

The free energy landscape near the phase boundary



➢H=0.01: the metastable minimum vanishes completely across all temperatures.

Relative variance of the equilibration time and self-averaging

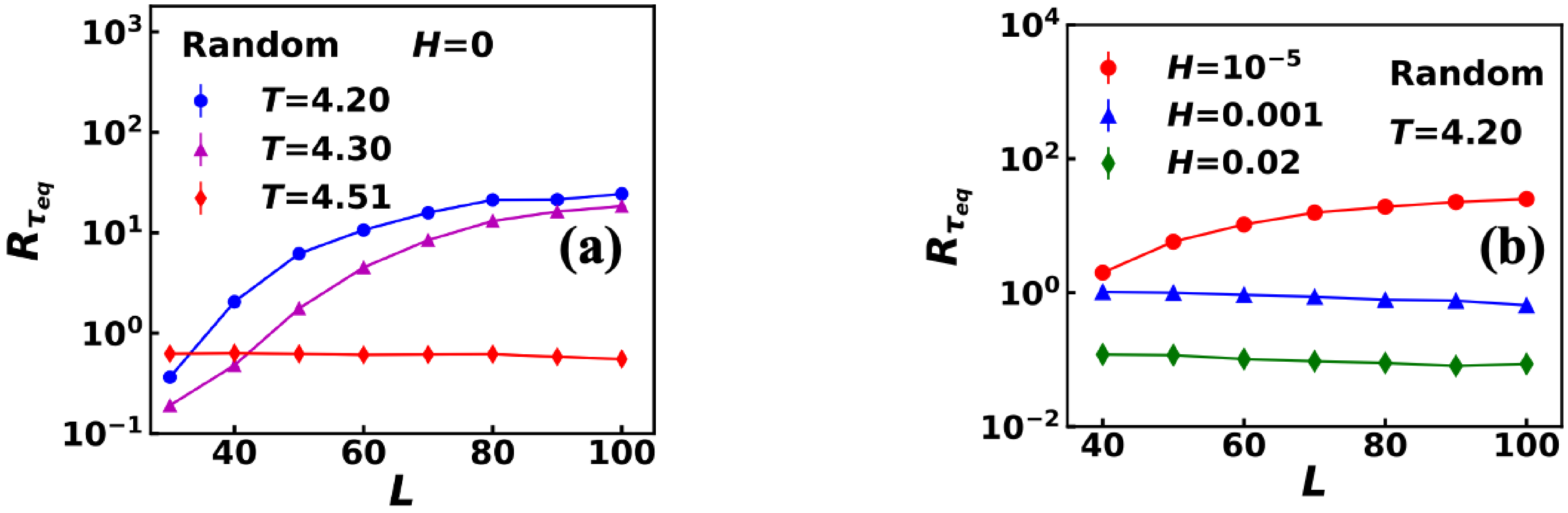
- The existence of coexistence states and metastable states at 1st-PT increases the randomness and uncertainty of the time evolution.

- To comprehensively understand the relaxation dynamics, the relative variance of τ_{eq} is defined as:

$$R_{\tau_{\mathrm{eq}}} = \frac{\overline{\tau_{\mathrm{eq}}^2} - \overline{\tau}_{\mathrm{eq}}^2}{\overline{\tau}_{\mathrm{eq}}^2}$$

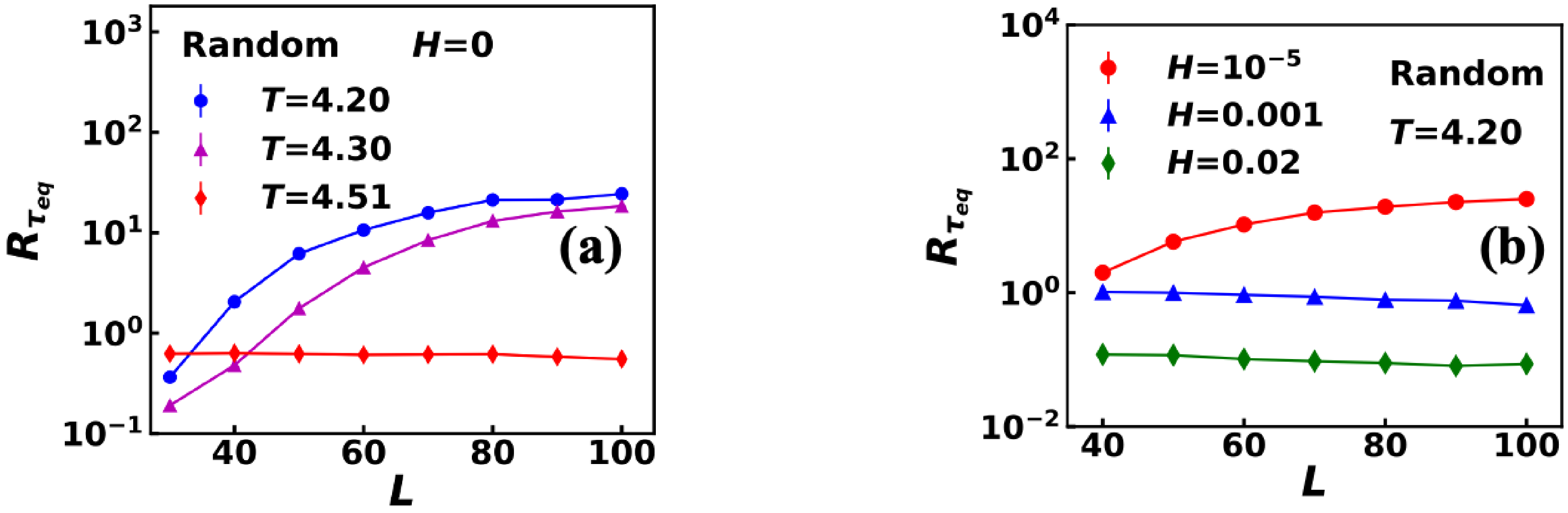
If $R_{\tau_{eq}}$ tends to zero as the system size increases, τ_{eq} is self-averaging.

$R_{\tau_{eq}}$ along the phase boundary



- For (a) : The $R_{\tau_{eq}}$ exhibits self-divergence at the 1st-PT line but non-self-averaging at the CP, revealing a previously unrecognized feature of the 1st-PT.
- For (b): The self-divergence characteristic of the 1st-PT disappears gradually when the system is away from the phase boundary.

$R_{\tau_{eq}}$ along the phase boundary



- The self-divergence behavior is observed not only at the 1st-PT line but also in its close vicinity.

Summary

- **Comprehensive free energy landscape**: We constructed the free energy landscape along the entire first-order phase transition line, which provides valuable insight into the relaxation behavior across the 1st-PT boundary.

- **Verification of ultra-slow relaxation**: Fine pre-equilibrium structures trap random initial states, further confirming the ultra-slow relaxation previously identified along the 1st-PT line.

- **New hallmark of 1st-PT**: The self-divergence of the relative variance of equilibration times reveals a previously unrecognized feature of first-order phase transitions.

Thanks to attention.