Free Energy Structure and Relaxation Characteristics Near the First-Order Phase transition Line

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Abstract

We study the relaxation dynamics of the three-dimensional kinetic Ising model along the phase boundary, focusing on the relaxation behavior [1] and the evolution of the underlying free-energy landscape[2]. We find that the average equilibration time increases significantly as the temperature moves far below the critical point T_c, and exhibits ultraslow relaxation along the first-order phase transition line. Dynamic scaling persists both near T_c and at $T_c \ll T_c$, with the latter showing a larger dynamic exponent. By tracking the time evolution of the free-energy landscape, we show that complex fine structures emerging at low temperatures trap random initial configurations, producing a strong delay in equilibration - the effect we identify as ultra-slow relaxation.This phenomenon is characterized by a self-divergence of the relative variance of equilibration times, revealing a previously unrecognized dynamic signature of first-order phase transitions.

Introduction

While critical relaxation has been well studied, the nonequilibrium dynamics along first-order phase boundaries are still not fully understood. In our recent work, we found an ultra-slow relaxation along the first-order transition line (1st-PTL), with equilibration times much longer than at the critical point. This strong slowing down may be related to the complex free-energy landscape, where stable and metastable states compete during the evolution.

Ising model

The 3D Ising model considers a simple cubic lattice composed of $N = L^3$ spins, where L is called the system size. The total energy of the 3D Ising model in a uniform external field H is expressed as:

$$E_{\{s_i\}} = -J\sum_{<ij>} s_i s_j - H\sum_{i=1}^{N} s_i,$$

Where J is known as the nearest-neighbor interaction constant between two spins s_i and s_j. The Free energy is evaluated by

$$F = -k_B T lnZ = -k_B T \sum_{\{s_i\}} e^{-\frac{E_{\{s_i\}}}{Nk_B T}}.$$

The structure of Free energy landscape along the entire phase boundary

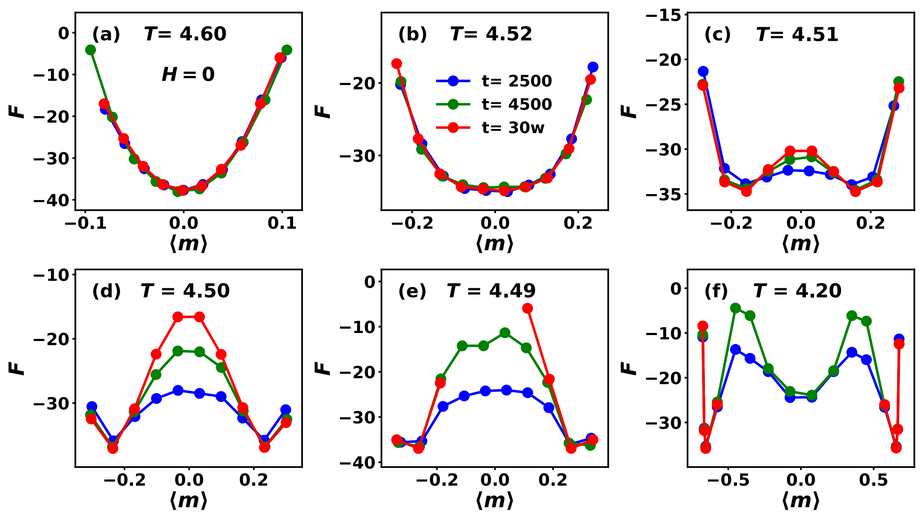

FIG.1 The free energy F as a function of the average order parameter $\langle m\rangle$ for six temperatures when $H = 0$ and lattice size $L = 60$.

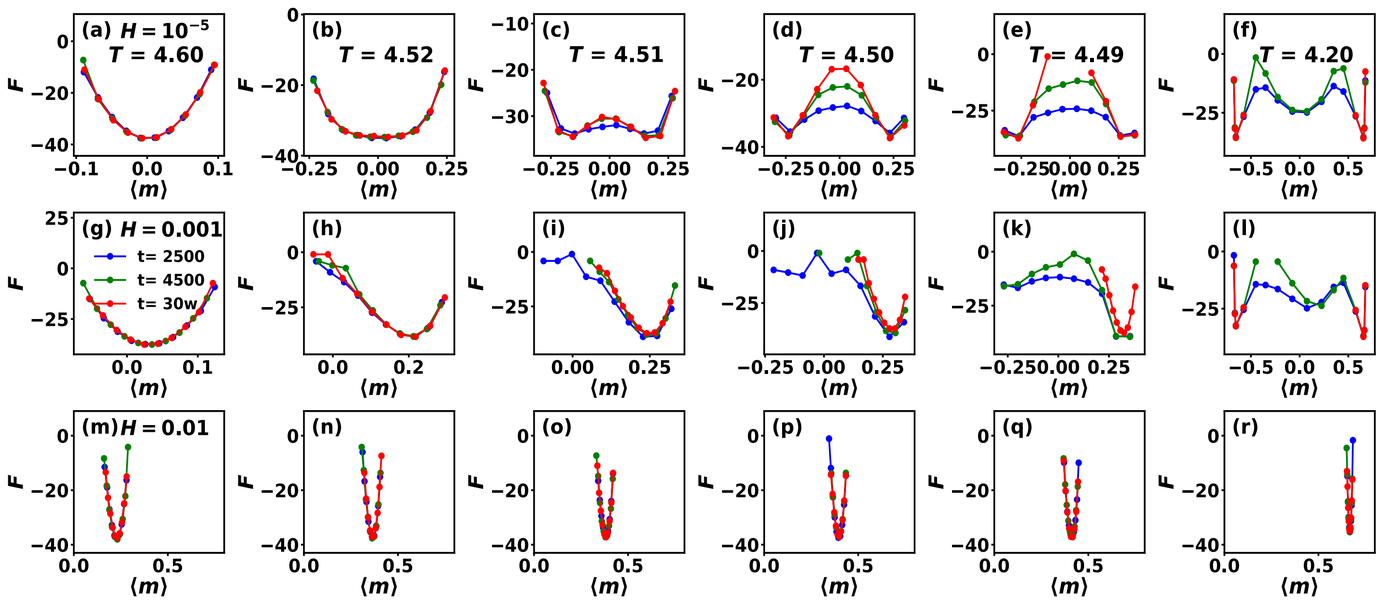

FIG.2 The free energy F as a function of the average order parameter $\langle m\rangle$ for six temperatures at three different external fields.

- Along the 1st-PTL, as the temperature decreases, the energy barrier between the two coexisting phases diverges.
- Along the phase transition line, the time required for the system to reach full stability becomes increasingly longer as the temperature decreases.
- As the external field increases, the system reaches full stability more quickly, and the metastable states gradually disappear.

The self-averaging properties of equilibrium time

The Self-averaging refers to the behavior of the relative variance of an observable X as the system size increases. It is defined as follows:

$$R_X = \frac{\overline{X^2} - \bar{X}^2}{\bar{X}^2},$$

where bar represents the average over the entire samples.

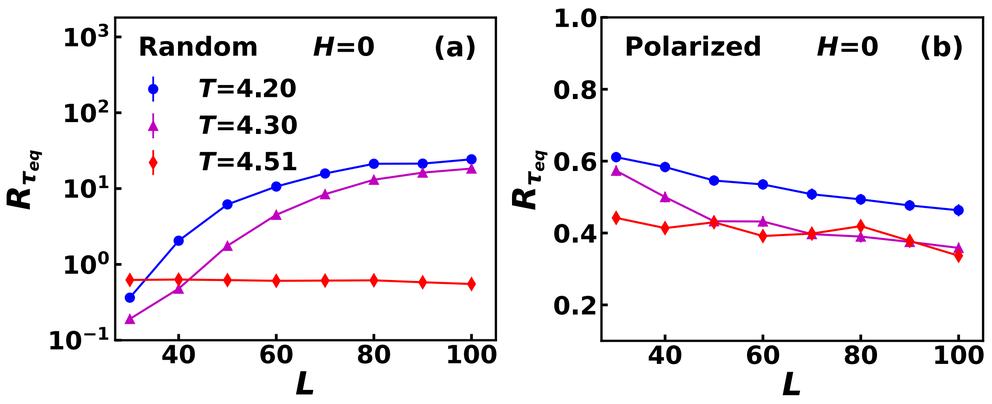

FIG.3 $R_{\tau_{eq}}$ as a function of L for different initial states: random initial state(a), polarized initial state(b.).

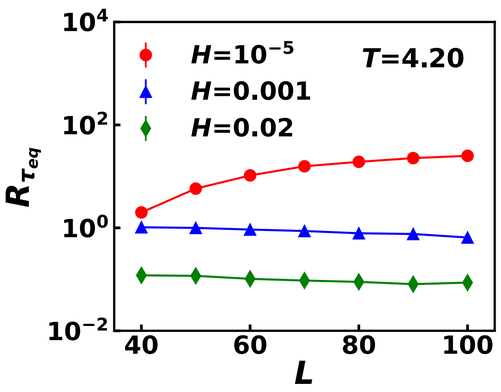

FIG.4 $R_{\tau_{eq}}$ as a function of L for three different values of the external magnetic field at $T = 4.20$.

- The self-divergence of the equilibrium time near the 1st-PTL directly reflects the increasing free energy barrier, indicating that the system evolves extremely slowly in this regime.
- In contrast, the non-self-averaging behavior of the equilibrium time near the critical point reflects the enhancement of fluctuations in the system.

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-PTL.
- **Verification of ultra-slow relaxation**: Fine pre-equilibrium structures trap random initial states, further confirming the ultra-slow relaxation previously identified along the 1st-PTL.
- **New hallmark of 1st-PT**: The self-divergence of the relative variance of equilibration times reveals a previously unrecognized feature of 1st-PTL.

[1]Phys. Rev. E 111, 064115 (2025). [2]arXiv: 2504.14878.