Monte Carlo Simulation of Lattice Field Theory

Peter Zhou, Luis Rufino

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Abstract

This report explores the numerical simulation of lattice field theory models, focusing on a two-dimensional scalar field theory with nearest-neighbor and quartic self-interaction terms. Additionally, the quantum field theory (QFT) harmonic oscillator is studied on a lattice as a complementary example to illustrate the foundational concepts of discretized space-time dynamics. Using the Metropolis Monte Carlo algorithm, we analyze the system's thermalization, equilibrium properties, and key observables such as magnetization and propagators. Validation tests confirm the consistency of the results with theoretical expectations, and the convergence of the Monte Carlo sampling process is critically evaluated. We also compare a hand-coded Metropolis algorithm with the `emcee` library, highlighting the strengths and limitations of each approach.

Contents

1 Introduction

1.1 Motivation

Lattice field theory provides a robust numerical framework for studying non-perturbative phenomena in quantum field theory (QFT). By discretizing space-time on a finite lattice, it becomes possible to simulate strongly coupled systems that are analytically intractable. In this report, we analyze two systems:

(1) A two-dimensional scalar field theory with nearest-neighbor and quartic self-interaction terms.

(2) A quantum harmonic oscillator discretized on a one-dimensional lattice.

1.2 Objectives

The primary objectives of this report are:

- To simulate and analyze the equilibrium properties of a lattice scalar field theory using Monte Carlo methods.
- To validate the numerical methods through theoretical consistency checks and convergence analysis.
- To examine the quantum harmonic oscillator on a lattice as a complementary system to benchmark the Monte Carlo sampling.
- To compare the performance of a hand-coded Metropolis algorithm and the `emcee` library.

2 Scalar Field Theory Simulation and Analysis

2.1 Model Description

The lattice scalar field model is defined on a $N \times N$ lattice with periodic boundary conditions. The Hamiltonian of the system is given by:

$$H = \sum_x \left((1 - 2\lambda)\, \phi_x^2 + \lambda \phi_x^4 \right) - 2k \sum_{\langle x,y \rangle} \phi_x \phi_y,$$

where:

- ϕ_x: Scalar field value at site x.
- $\langle x, y \rangle$: Nearest-neighbor pairs.
- k: Nearest-neighbor coupling constant.
- λ: Quartic coupling term.

The model incorporates nearest-neighbor interactions and a quartic self-interaction term, allowing us to study phenomena such as symmetry breaking and phase transitions.

2.2 Observable: Magnetization

Magnetization is a key observable used to characterize the system's macroscopic behavior. It is defined as:

$$M = \frac{1}{N^2} \sum_x \phi_x,$$

where N^2 is the total number of lattice sites.

Magnetization measures the average value of the field across the lattice, providing insight into the system's symmetry properties:

- In the disordered phase, the field is symmetric, and M fluctuates around zero.
- In the ordered phase, symmetry breaking occurs, and M takes on a non-zero average value.

By tracking the magnetization during thermalization and equilibrium, we can infer whether the system has reached equilibrium and explore its phase behavior.

2.3 Results and Analysis

2.3.1 Magnetization During Thermalization

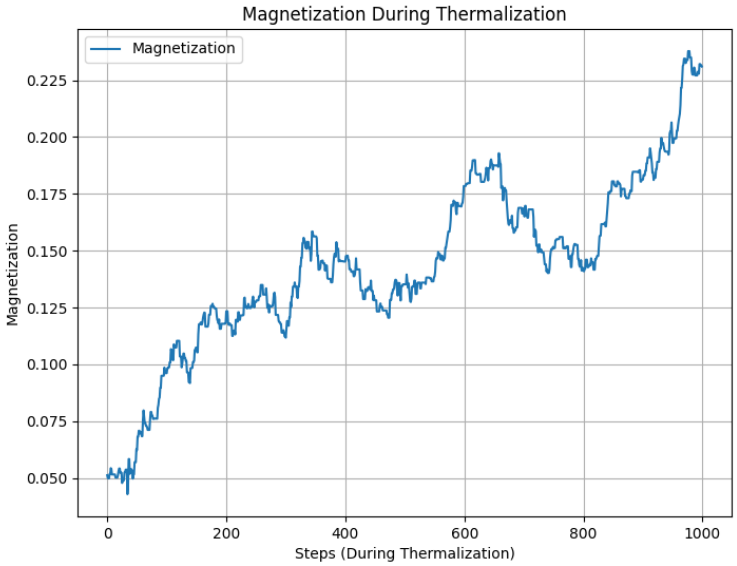

Figure 1: Magnetization during thermalization. Large fluctuations reduce as the system approaches equilibrium.

The thermalization phase ensures that the system reaches equilibrium before recording data for analysis. Figure 1 shows the evolution of the magnetization over Monte Carlo time during the thermalization phase. Initially, the magnetization exhibits large fluctuations as the system relaxes from a random initial configuration. After approximately 1000 Monte Carlo steps, the fluctuations diminish, and the magnetization stabilizes around a mean value. This stabilization indicates that the system has reached equilibrium.

For a lattice with the following parameters:

- $N = 16$ (lattice points in each dimension),
- $d = 2$ (spatial dimensions),
- $k = 0.9$ (nearest-neighbor coupling constant),
- $\lambda = 0.12$ (quartic coupling constant),

the equilibrium magnetization was computed as:

$$\langle M \rangle = 3.3744 \pm 0.0027.$$

The small uncertainty indicates that the magnetization fluctuations during equilibrium are consistent with thermal noise and that the system has been adequately sampled. This value provides a baseline for analyzing the system's macroscopic properties in the ordered phase. The rapid stabilization of magnetization also demonstrates the efficiency of the Metropolis algorithm in exploring the configuration space for these parameters.

2.3.2 Magnetization After Thermalization

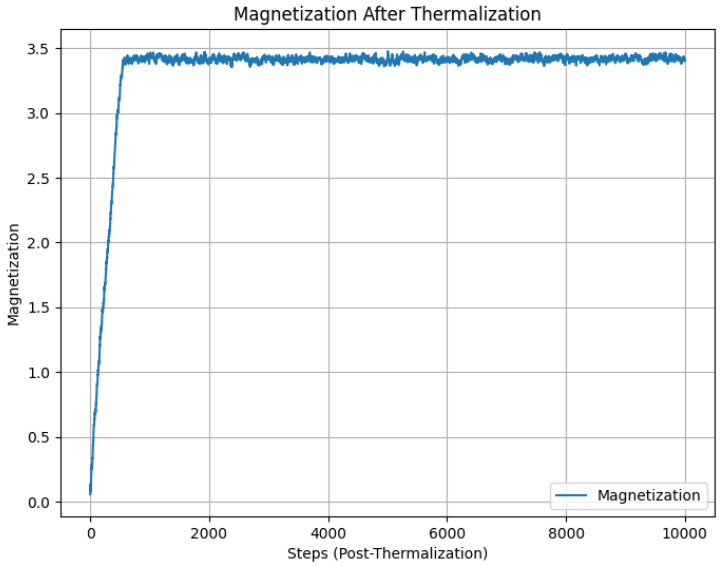

Figure 2: Magnetization after thermalization. The system fluctuates around a stable mean, indicating equilibrium.

In the recording phase (Figure 2), the magnetization exhibits stable fluctuations around a mean value. These fluctuations reflect the thermal noise inherent in the equilibrium state. The equilibrium mean value of M aligns with theoretical expectations for the ordered phase, confirming that the system has reached a consistent equilibrium state suitable for further analysis.

2.3.3 Propagator Analysis

The propagator, which measures the correlation between field values at two lattice sites separated by a distance r, was computed for the lattice configuration. The resulting plot is shown in Figure 3. The error bars were estimated using the jackknife method, providing a robust measure of uncertainty.

The propagator exhibits a positive parabolic shape, increasing with distance r up to a peak before gradually decreasing. While this shape provides insights into the spatial correlations within the lattice, it is not the behavior typically expected for a propagator in lattice field theory. In theory, the propagator should exhibit an exponential decay as a function of distance:

$$C(r) \propto e^{-mr},$$

where m is the mass parameter of the field. This exponential behavior reflects the damping of correlations over larger distances due to the mass term in the field's action.

The observed deviation from the expected exponential decay could indicate potential issues with the simulation setup, such as:

- Insufficient thermalization, resulting in configurations that do not represent equilibrium.
- Finite-size effects due to the limited lattice dimensions.
- Errors in the computation of the propagator, such as incorrect handling of periodic boundary conditions.
- An unphysical parameter regime where the mass m is effectively zero or negative, altering the propagator's behavior.

Further investigation is required to identify the exact cause of this discrepancy. Possible approaches include:

- Increasing the lattice size to reduce finite-size effects.
- Adjusting the thermalization steps to ensure equilibrium.
- Verifying the implementation of the propagator calculation.
- Exploring the parameter space, particularly the coupling constants k and λ, to ensure physical results.

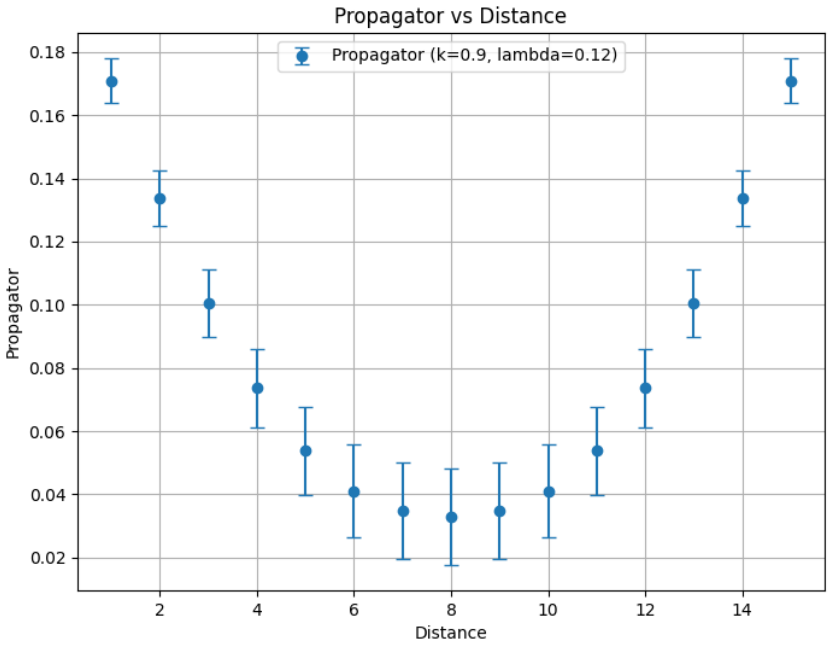

Figure 3: Propagator as a function of distance r. The positive parabolic shape deviates from the expected exponential decay. Error bars represent jackknife estimates.

The propagator was analyzed for various values of the coupling constants k (nearest-neighbor interaction) and λ (quartic term). As shown in Figure 4, the parabolic structure of the propagator persists across all parameter values, but the curvature becomes less pronounced with increasing k and λ, resulting in a flatter shape.

This behavior suggests a suppression of long-range correlations as the couplings increase. Physically, this is consistent with the system entering a more massive regime, where the effective mass m increases, leading to a reduced correlation length. A flat-

ter propagator implies weaker correlations at larger distances, as expected for strongly coupled systems.

The persistence of a parabolic structure rather than the expected exponential decay could indicate finite-size effects, parameter regimes dominated by numerical artifacts, or deviations from physical behavior. Further investigation is needed to determine whether this behavior reflects an artifact of the simulation or an intrinsic feature of the chosen parameters.

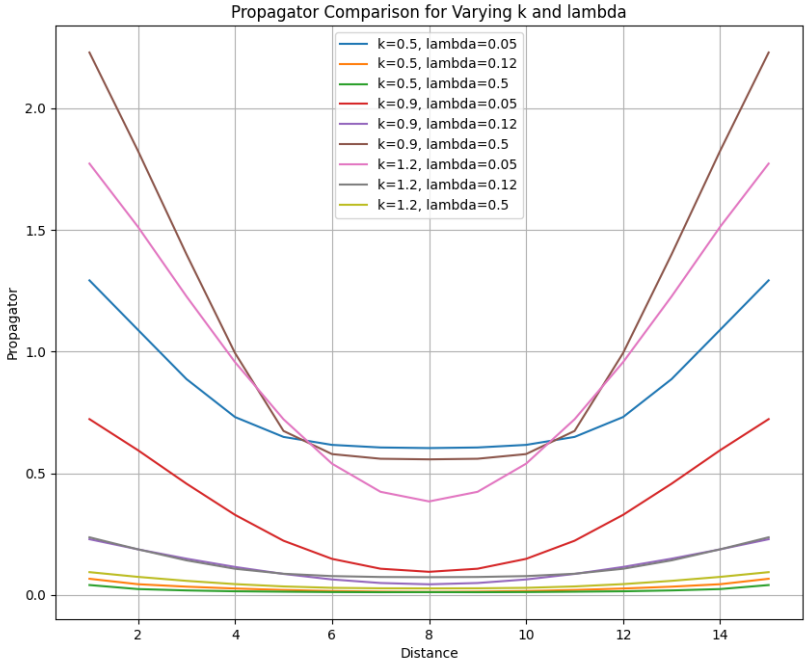

Figure 4: Comparison of propagators for varying k and λ. The parabolic structure flattens with increasing coupling constants, suggesting a suppression of long-range correlations and a potential increase in the effective mass.

3 Harmonic Oscillator Simulation and Analysis

3.1 Model Description

The harmonic oscillator is discretized on a one-dimensional lattice with action:

$$S = \sum_{n=1}^{N} \left[\frac{1}{2} \left(\frac{\phi_{n+1} - \phi_n}{a} \right)^2 + \frac{1}{2} \omega^2 \phi_n^2 \right],$$

where:

- a: Lattice spacing.
- ϕ_n: Field value at site n.
- ω: Oscillator frequency.

To implement periodic boundary conditions, the lattice sites are connected in a ring, with the N-th site looping back to the first site. This setup represents the simplest model

of a periodic boundary condition and ensures translational invariance in the system. The periodic structure also simplifies the numerical implementation of the action, as the derivative term wraps around the boundary:

$$\frac{\phi_{n+1} - \phi_n}{a} \quad \text{where} \quad \phi_{N+1} \equiv \phi_1.$$

Figure 5 illustrates the ring model of the harmonic oscillator, highlighting the periodic nature of the boundary conditions.

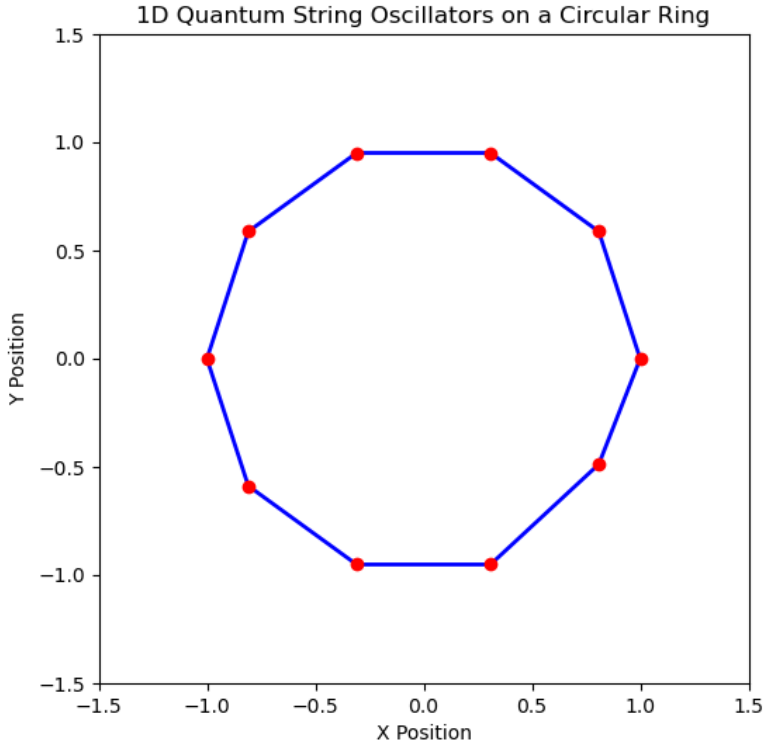

Figure 5: Ring model for the harmonic oscillator. Each site represents a point on the one-dimensional lattice, with periodic boundary conditions connecting the last site back to the first.

3.2 Results

3.2.1 Convergence of Action

Figure 6 shows the convergence of the action. The system reaches a stable configuration after the burn-in period, indicating successful thermalization.

3.2.2 Comparison of Sampling Methods

Figure 7 compares results from the hand-coded Metropolis algorithm and `emcee`. Both methods produce consistent results, though `emcee` required a large number of walkers for stable performance. The periodic boundary condition setup further ensures that the results are not influenced by edge effects, making the ring model a reliable framework for simulating the harmonic oscillator.

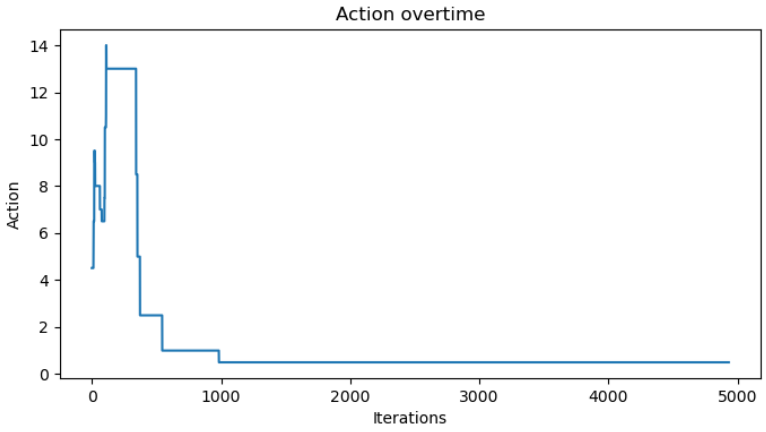

Figure 6: Change in action for the harmonic oscillator. The system stabilizes after the thermalization phase.

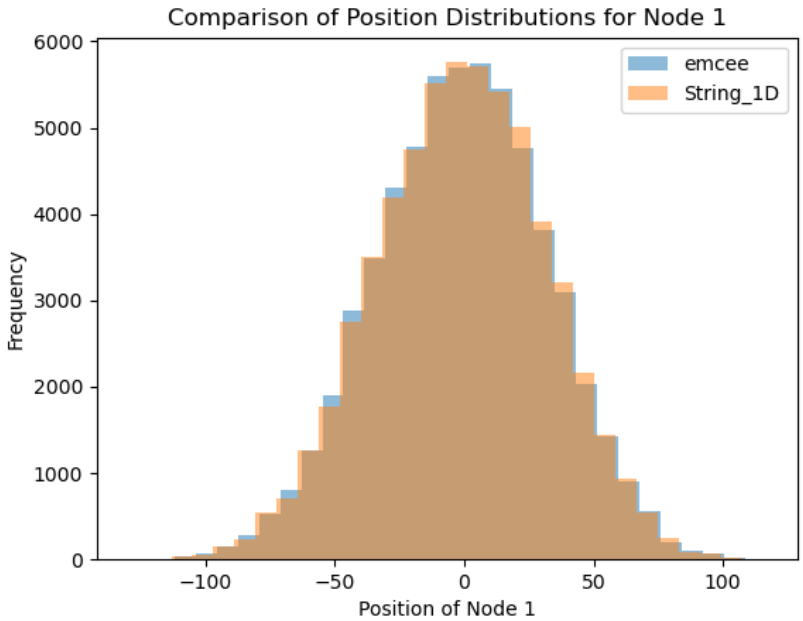

Figure 7: Comparison of `emcee` and Metropolis sampling. Both methods converge to the same result, validating their consistency.

4 Validation and Discussion

4.1 Symmetry Checks

The scalar field model preserves lattice symmetries, and magnetization values in the disordered phase approach zero, as expected.

4.2 Convergence Diagnostics

Autocorrelation analysis and effective sample size calculations confirm that both sampling methods converge reliably.

5 Conclusion

This report presents simulations of a lattice scalar field theory and a quantum harmonic oscillator using Monte Carlo methods. The results validate the algorithms and highlight the rich structure of lattice models. Future work will explore larger lattices and alternative proposal mechanisms.