MCMC simulation of ergodic lattice field theory

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1 Abstract

Starting from the end of 20th century, the strong coupling regime of Quantum Field theory has drawn great attention in theoretical physics. Some systems like ϕ^4 has being investigated in depth through a set of method of non-linear lattice field theory, but it was all based on dynamical formulation in which dynamic happens in the forward in time direction, making it computationally expensive. Recently, Liang and Cvitanović (Han Liang, 2022) proposed a spatiotemporal formulation of non-linear field theory that describes a system globally through periodic solutions. We aim to test several aspects of this new formulation through Markov Chain Monte Carlo (MCMC) simulation. Our result gives a positive feedback on the correspondence between zeta function and partition function, as well as a moderate support on the convergence of zeta function (whose effects are weakened by random fluctuation). This would be a good example of how simulation can add on to the frontier of theoretical physics, in the regimes well beyond any the govern of any classical law. There could be more creative ways to include simulations in the study of field theories that can bring new energy into this subject.

2 Introductory material

In this project, we aim to test a new formulation of non-linear field theory based on MCMC simulation. As the main purpose is to check the validation of a theoretical formulation, the purpose and interpretation of results from the simulation would be naturally different from main stream fluid simulation. We will begin by an introduction of this highly theoretical topic.

In spatiotemporal formulation, a scalar field $\phi(x)$ over d Euclidean coordinates can be discretized by replacing the continuous space by a d-dimensional hypercubic integer lattice $\mathbb{Z}^d$, with lattice spacing a, and evaluating the field only on the lattice points

$$\phi_z = \phi(x) \quad x = az, \;\; z \in \mathbb{Z}^d \tag{1}$$

A field configuration (here in one spatiotemporal dimension)

$$\Phi = ...\phi_{-2}\phi_{-1}\phi_0\phi_1\phi_2... \tag{2}$$

takes any set of values in system's ∞ -dimensional state space $\phi_z \in \mathbb{R}$. Consider a system with action defined as

$$S[\Phi] = \sum_z \{\frac{1}{2}\partial_\mu\phi_z\partial^\mu\phi_z + V(\phi_z)\} \tag{3}$$

$$= \sum_z \{\frac{1}{2}\phi_z\Box\phi_z + V(\phi_z)\} \tag{4}$$

where $\Box$ is Laplacian

$$\Box\phi_z = \sum_{||z-z'||=1} (\phi_{z'} - \phi_z) \tag{5}$$

Specifically, we are interested in the 1-dimensional ϕ^4 theory, where potential function is an even quartic function.

$$V(\phi_z) = -\frac{\mu^2}{4}\phi_z^4 + \frac{\mu^2}{2}\phi_z^2 \tag{6}$$

In a 1-dimensional theory, standard state space is $\mathbb{R}^2$, and we replace the spatiotemporal index z by temporal index t. The resulting Euler-Lagrange equation reads

$$-\phi_{t+1} + 2\phi_t - \phi_{t-1} + \mu^2(-\phi_t^3 + \phi_t) = 0 \quad \forall t \in \mathbb{Z} \tag{7}$$

To see that the state space is indeed $\mathbb{R}^2$, it's easier to adopt Hamiltonian formulation

$$\begin{bmatrix}\phi_{t+1}\\ \phi_t\end{bmatrix} = \begin{bmatrix}-\mu^2\phi_t^2 + (\mu^2+2) & -1\\ 1 & 0\end{bmatrix}\begin{bmatrix}\phi_t\\ \phi_{t-1}\end{bmatrix} \tag{8}$$

or simply forward in time formulation

$$\phi_{t+1} = -\phi_{t-1} - \mu^2\phi_t^3 + (\mu^2+2)\phi_t \tag{9}$$

This Euler-Lagrange equation has only one parameter μ^2, the Klein-Gordon mass, due to energy renormalisation equivalence (by simply scaling ϕ to get a new by equivalent field theory for ϕ'), and this Klein-Gordon mass represents the strength of coupling. For a strong enough coupling, this system is what called a hyperbolic system, and the dynamics of this system is topologically equivalent to a 3-symbol full shift, meaning that the set of bi-infinite 3-symbol string is in one-to-one correspondence with admissible orbits of this system (by admissible we mean bounded in usual metric of $\mathbb{R}^2$). This makes numerical methods very powerful in calculation of periodic orbits for such a system.

However, nothing can come with no cost. When it comes to hyperbolic system, all information is contained in a non-wandering set (the set of all admissible

orbits), and this set is a fractal for any open system like ϕ^4 theory. Usually, expectation value of observable a is defined by Birkhoff's ergodic theorem as

$$\langle a \rangle = \lim_{n\to\infty} \sum_{k=0}^{n} a(f^k(x)) \tag{10}$$

for almost all points x in the non-wandering set (except for a zero-measure subset which includes all periodic solutions). For an open system, all points in an open set escapes at exponential rate, which means that we can never find a representative point x in the non-wandering set. All the randomly guessed points escape this system at some constant rate (escape rate of the system) after each iteration, leaving exponentially fewer points, which makes it impossible to calculate expectation by directly following an ergodic orbit (although its existence is mathematically proven). Thus, lots of efforts has been put into the search of a method to calculation expectations of ergodic systems like these. Our goal is to simulate an ergodic solution and use that to calculate expectation value.

Liang and Cvitanović (Han Liang, 2022) proposed a method of calculating expectations in ergodic field theories, using periodic orbits as skeleton and push the calculation globally. In fact, it follows the same philosophy of individual training process for solving differential equation by neural network, globalizes local differential equation to Euler-Lagrange equation (9). A solution is obtained by minimizing this global loss given by the loss of (9) using gradient descent method.

The full power of this global point of view is revealed by partition function and zeta function, which are both based on periodic solutions. This method can be easily generalize the higher spatiotemporal dimensional. For a given tiling $\mathbb{A}$ of state space, the partition function of an integrable observable a is defined as

$$Z_{\mathbb{A}}(\beta) = \sum_c \frac{1}{|\mathrm{Det}\mathcal{J}_c|} e^{V_{\mathbb{A}}\langle a\rangle_c \beta} \tag{11}$$

where $V_{\mathbb{A}}$ denotes the volume of prime cell, c is a periodic state such that $\mathbb{A}$ gives a periodic tiling of c, and $\mathcal{J}_c$ is the orbit Jacobian matrix related to state c, which represents orbit stability. Integrated over the prime cell $\mathbb{A}$, stability $1/|\mathrm{Det}\mathcal{J}_c|$ is replaced by the stability exponent $e_{-\lambda_c} V_{mathbbA}$, and the sum is thus

$$Z_{\mathbb{A}}(\beta) = \sum_c e^{V_{\mathbb{A}}(\langle a\rangle_c \beta - \lambda_c)} \tag{12}$$

Acute mind suddenly notice that (12) is a geometric series of $V_{\mathbb{A}}$, so a invention of generating function of all partition functions is natural at this point

$$Z[\beta, z] = \sum_{\mathbb{A}} Z_{\mathbb{A}}(\beta) \frac{z^{V_{\mathbb{A}}}}{V_{\mathbb{A}}} \tag{13}$$

This sum is then transformed into a sum of prime orbits, which is a smaller counting index as it avoid n-time overcounting of a period-n state n times. An orbit p will appear in the sum $\mathbb{A}$ each time $V_{\mathbb{A}}$ is a multiple of V_p in all dimensions, and the previous some becomes

$$Z[\beta, z] = \sum_p \sum_{n=1}^{\infty} \frac{1}{n} e^{nV_p(\langle a \rangle_p \beta - \lambda_p)} z^{nV_p} = -\sum_p \ln(1 - t_p) \tag{14}$$

where $t_p[\beta, z] = e^{V_p(\langle a \rangle_p - \lambda_p)} z^{V_p}$. Zeta function is defined by relation $\zeta = \mathrm{Z}$, which is naturally in product form

$$1/\zeta[\beta, z] = \prod_p (1 - t_p) \tag{15}$$

Expectation value of a is calculated by partition function (12) as

$$\langle a \rangle = \left. \frac{\partial}{\partial \beta} \right|_{\beta=0} \ln Z = \sum_c \frac{1}{|\mathrm{Det} \mathcal{J}_c|} \langle a \rangle_c \tag{16}$$

and zeta function evaluation is similar

$$\langle a \rangle = \left. \frac{\partial}{\partial \beta} \right|_{\beta=0} \ln \zeta = \sum_p \frac{T_p}{|\Lambda_p| - 1} \langle a \rangle_p \tag{17}$$

where $|\Lambda_p|$ is product of all expanding eigenvalues of Jacobian matrix for p. Both sums are formal sums with infinite terms, which inspires us to evaluate them by MCMC simulation. In fact, this zeta function seems to have some problem of normalization due to its slow convergence rate. Thus, this project is devoted to evaluate both (16) and (17) and check their correspondence by MCMC simulation.

The first part of the project is to reproduce this calculation using so called shadow state method and gradient decent, but with better efficiency on the identification of prime orbits (which are periodic orbits that are not repeats of a shorter orbit and quotient by cyclic permutation symmetry). The second part is to parallelize the calculation of zeta function coefficients, which should enable us to push the current precision limit by a few digits (now limited by calculation time). And the final part is to use MCMC to simulate an ergodic orbit in this system and directly calculate its corresponding expectation to compare with results from zeta function. Once worked out, it would be an important justification of the lattice formulation for field theories. (M. S. Albergo & Shanahan, 2019)

3 Methods

As partition function and zeta function are both based on periodic solution, it is important to have a function that generate periodic states. The set of all these

states can be thought as the state space of Markov Chain. Thus, the first step is to find the periodic states for this system and extract from them the prime orbits (for zeta function). The first part is preliminary, with the shadow states given by symbolic dynamics and exact solution found by gradient descent. All of these are presented as the package called cyclehunter.

In cyclehunter, solutions are found by descending from its initial guess given by shadow states. Each shadow state is given by the symbolic dynamics of that identifies the periodic state. Thus, to generate the set of all period-n solutions, the first step is to generate all length-n symbol strings and then turn them into shadow states. To extract prime orbits, it is more convenient to extract all of their symbol strings. This method is included in cyclehunter, but it is way too inefficient that limited the previous calculation to only period 10. Thus, the first part of this project is to develop a new algorithm that extracts prime orbits more efficiently.

To understand this algorithm, it is important to first understand periodic states and prime orbits. For any hyperbolic system abovementioned, periodic states and symbol strings are in one-to-one correspondence. For example, ϕ^4 theory as three symbol (call them "-1", "0", "1"), and a period-two state is given by "0 1" or "-1 0" or "0 0" etc., while the last one is just a twice repeat of a fixed point "0". The set of all prime orbits, by its essence, is the set of all periodic states quotient by symmetric group of the system. For example, a general periodic state with period $2n$ naturally has $2n$ copies, related by cyclic permutation, and it is also possible that it is a twice repeat of an orbit with period n. A prime orbit is to quotient all of the cyclic permutation and repeats.

The algorithm for prime orbits is illustrated by Figure 1. If we have N period states, then the old method is $\mathcal{O}(N^2)$ in time complexity, and the new algorithm, as set search is $\mathcal{O}(1)$, is $\mathcal{O}(N)$. Since the number of periodic states grows exponentially as period goes longer, this $\mathcal{O}(N^2)$ drives the calculation crazy. Thus, instead of pairwise comparison (with doubled length to identify repeats of periodic states with shorter period), we developed a encoding system. Every state is expanded as a group-theoretical orbit given by the symmetric group we want to quotient, and then each element is encoded by ternary expansion and added to a set. The size of this temporary set is the length of the group theoretical orbit, and if it doesn't equal to the period, then it means the orbit considered is a repeat of a shorter one. If not, then we take the minimum of this temporary set and search whether is minimum (as the unique code of a prime orbit) has already been added to the set of all prime orbits. With the new algorithm developed, we can push the limit of period length from 10 to 14 now, which is already enough for our simulation.

With all the prime orbits found, simulation is almost ready. For recycling purpose, we put all the prime orbits calculated in a txt file and write it into a dictionary whenever we need to use them. Keys are integers, and values are field values for corresponding prime orbits. We found it more efficient than putting them into a list, in terms of space complexity. Then, the Markov chain is a hopping between states labeled by integers.

As we are simulating ergodic solutions in many different cases (with different

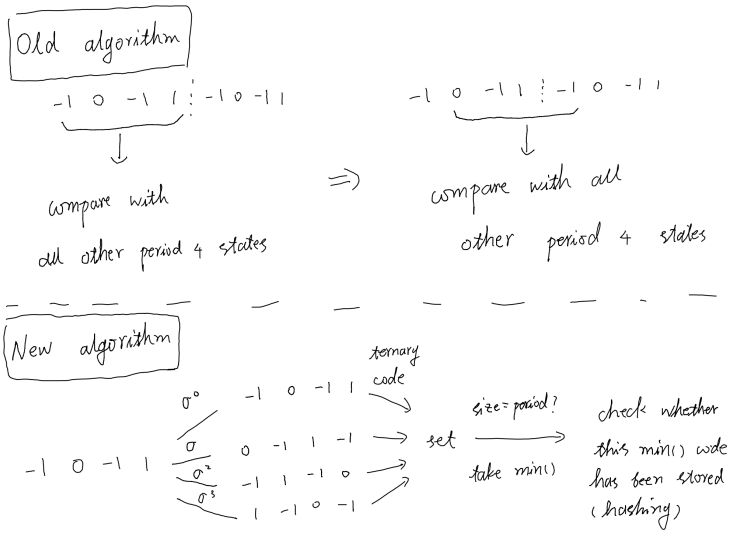
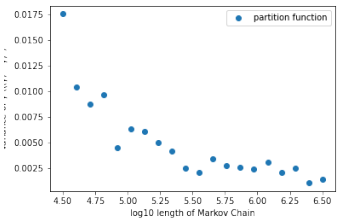


Figure 1: An illustration of algorithms for prime orbit extraction (both old and new algorithm are included)

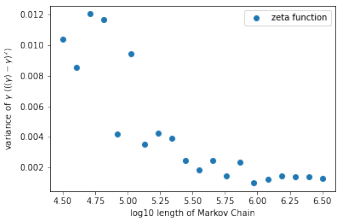
lengths and different size of state space to check convergence), each simulation is independent. Thus, it would be the most efficient if simulations are parallelized and then use a manager to collect all the results.

The setup for MCMC simulation would be more complicated. Similar to the partition function of a system with infinite states, this zeta function is built up by infinitely many periodic orbits. Thus, it is necessary to employ Metropolis algorithm (Newman, 2021) to simulate the ergodic solution (which can be understood as the solution that visits every part in the state space). The transition probability is given by ratios of stability of two orbits, but the convergence rate is yet to be worked out. The quantities we what to inspect is the average stability, as it would be related to escape rate of the open system, which should be straight forward to calculate analytically by zeta function (which we are devoting to do). This yields the first drawback of our method: there is no reference value to compare to. It won't affect the correspondence between zeta function and partition function, neither the test of how truncation could affect zeta function expectation, but without an reference value it does not fulfill the goal to 'test the theory by simulation'.

One final goal was to employ this simulated ergodic solution to generate a natural measure (invariant under time evolution) of the non-wandering set, which is related to this ergodic solution by Birkhoff's ergodic theorem (Birkhoff, 1931). However, as this method is solely based on periodic solutions, it is impossible to test evolution invariance, which is trivial for any periodic solution. Thus, this is still far from a perfect bridge to strict ergodicity.



(a) Variance v.s. chain length for partition function



(b) Variance v.s. chain length for zeta function

Figure 2: Test of convergence by variance of repeated simulations

4 Results

First, we check that our simulation result converges to a specific value. To this end, we calculate the variance of ten repeated simulation with the same setup (i.e. same length of Markov chain). The result is shown in Figure 2

The variance for both zeta function and partition function decrease to zero accordingly, which means that simulation at least converges to some value. The next step is to check the correspondence between zeta function and partition function. This result is shown is Figure 3

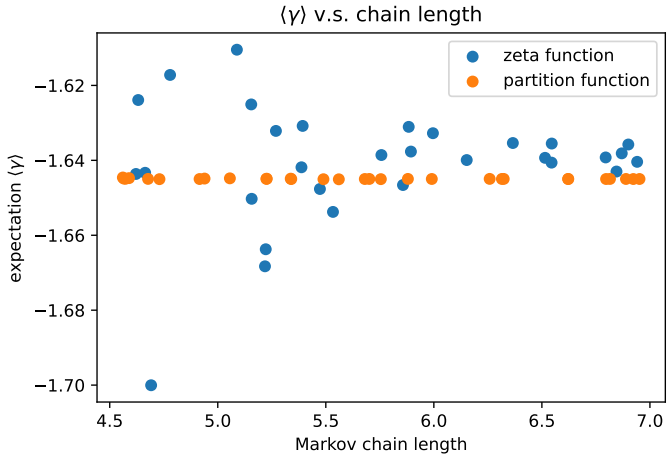


Figure 3: A plot of Markov chain length v.s. expectation value for both partition function (period 13) and zeta function (prime orbit up to period 12)

A surprising fact is that expectation value calculated from partition function converges very fast regarding chain length (although there are more than 10^6 of them). To check that it is not a trivial value, we plot in Figure 4 the result

of partition function alone (a selected part of Figure 3). We can see that it is not trivial, but the variance is negligible compare to that of zeta function. The reason behind this is that the stability exponent we computed shows a high correlation with period, while 13 is a decently large prime number, which means that almost all periodic states with period 13 are not repeat of any shorter orbit. This makes the difference stability exponent for different states small, and thus the result turns out to be stable.

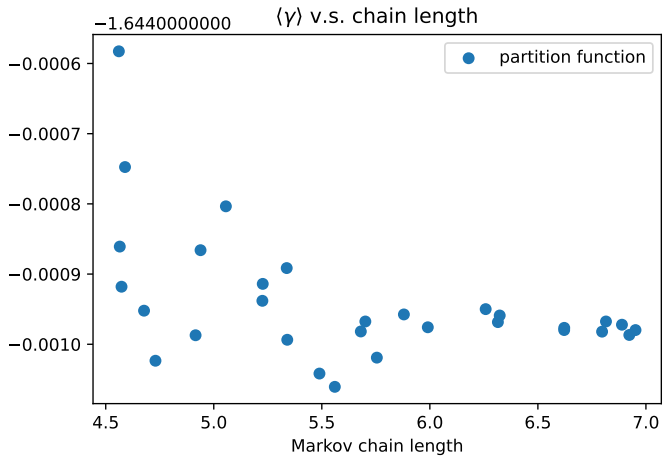


Figure 4: A plot of Markov chain length v.s. expectation value for partition function (period 13), local zoom out for Figure 3

As shown in Figure 3, although zeta function shows a much large variance, the expectation values from zeta function and partition function agrees with each other in an acceptable degree. As the state space of zeta function (prime orbit with period up to 12) and partition function (periodic states with period 13) has almost no overlap, we are confident to conclude that this test for the correspondence between zeta function and partition function is successful at this stage.

However, inspired by the pattern shown in Figure 3, we want to push the test one step further. Since partition function gives a generally stable value, we adopt it as the reference value (take $\langle\gamma\rangle = -1.6439$) and check how quickly zeta function result converges to this reference value. The theoretical prediction is that error should be exponentially decreasing as the length of period increases. The number of prime orbits also increases at exponential rate with period length, so we understand it as the logarithm error should decrease linearly with logarithm of size of state space (i.e. the number of prime orbits included in the simulation). To control variable, we fix Markov chain length at 10^7. This produces huge amount of calculation, which makes parallelization calculation necessary. The result is shown in Figure 5. We can see that despite of the random fluctuation (especially toward the end), there is a linear decreasing

trend. Thus, as the error itself and variance are at similar order of magnitude (even with Markov chain length 10^7), we cannot conclude that the result is a strong backup of the theory for zeta function convergence, but at least they agree in a satisfactory degree.

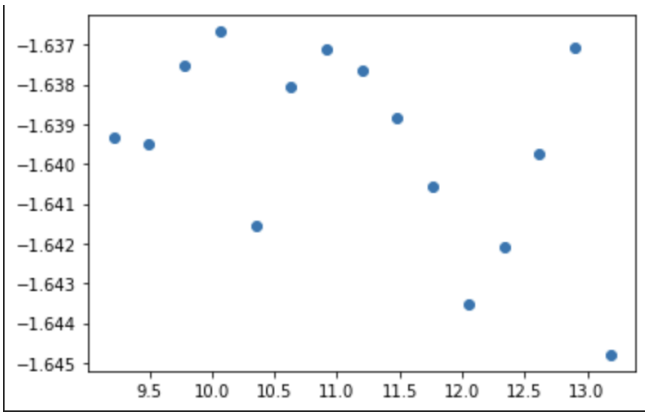


Figure 5: A plot of state space size (logarithm) v.s. error (logarithm) with Markov chain length fixed at 1e7

5 Conclusion

In this project, we tested several aspects of spatiotemporal formulation of lattice field theory based on MCMC simulation. As all the calculation were previously limited by the algorithm of identifying prime orbit, we developed a new algorithm that successfully reduced the complexity from $\mathcal{O}(N^2)$ to $\mathcal{O}(N)$ and extended the longest period from 10 to 14. For the main part, we used Metropolis algorithm to simulate an ergodic solution and used it to calculate expectation of stability based on zeta function and partition function. The results are shown in Figure 3. As the expectation from partition function is relatively stable, we pushed the test one step further to use the result from partition function as the reference value and calculated the convergence of zeta function. However, due to random fluctuation (even if we fixed chain length 1e7 and accelerated by parallelization), result in Figure 5 does not show a clear linear relation, but it still gives us some confidence that if we can further increase the chain length, there could be a promising linear relation.

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