Simulating the Double Well,
or,
A Metropolitan Adventure

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1 Introduction

Trying to do lattice Monte Carlo for the simplest possible quantum mechanical system with non-perturbative phenomena: the double well potential. The Euclidean action we consider is

$$S = \int dt \left(\frac{1}{2}\dot{x}^2 + \frac{1}{2}m^2 x^2 + \frac{1}{4}g^2 x^4 \right) , \tag{1}$$

with m^2 any real value (but we shall be most interested when it is negative) and g^2 a positive coupling. In abuse of terminology we will call m the mass in connection with field theory.

Since both parameters of the theory are dimensionful, we can form the dimensionless quantity

$$\alpha = \frac{m^2}{g^{4/3}} , \tag{2}$$

which we can think of as an inverse coupling. When $\alpha \gg 0$, the theory is weakly coupled about the origin. When $\alpha \ll 0$, the theory experiences spontaneous symmetry breaking and is again weakly coupled around each VEV. The elementary excitation has mass

$$\mu^2 = -2m^2 , \tag{3}$$

while the action of the instanton connecting the two VEVs is

$$S_{\text{inst}} = \frac{4}{3\sqrt{2}} \frac{m^3}{g^2} = \frac{4}{3\sqrt{2}} (-\alpha)^{3/2} . \tag{4}$$

In the intermediate strongly coupled region however, instanton processes become unsuppressed and the nature of the theory is unclear.

2 A Toy Example

To better understand the above theory, let us further simplify to a system without a kinetic term, only a single potential term, and discretized to the lattice:

$$S = a\, \Delta t \sum_{i}^{N} x_i^k . \tag{5}$$

Since the field values at each lattice point are uncoupled, we can easily compute the partition function

$$Z(\beta) = \int dx e^{-\beta S} \quad \sim \frac{1}{(\beta\, a\, \Delta t)^{N/k}} \tag{6}$$

where β is a fictitious inverse temperature that we shall set to 1. Consider the quantity

$$\langle S \rangle = - \frac{\partial \log Z}{\partial \beta}\bigg|_{\beta=1} \quad = \frac{N}{k}\,. \tag{7}$$

When we take $k = 2$ and think of S as a statistical mechanical energy, this reflects the well-known fact that each quadratic degree of freedom has energy $\frac{1}{2}T$. More generally, this equation reflects the fact as the exponent of (5) increases, the particle spends an increasing amount of time in the region with low action.

Bringing the toy model closer to (1), consider the (still decoupled) lattice action

$$S_0 = \Delta t \sum_i^N \left(\frac{1}{4}\theta(-m^2)\frac{m^4}{g^2} + \frac{1}{2}m^2 x^2 + \frac{1}{4}g^2 x^4 \right)\,. \tag{8}$$

The "0" subscript indicates that a constant term has been added to ensure that the global minimum of the action is 0. One can analytically compute the action per lattice site, obtaining

$$\frac{\langle S_0 \rangle}{N} = \frac{1}{4} + \gamma^2 \left[-1 + \frac{K_{3/4}(\gamma^2)}{K_{1/4}(\gamma^2)} \right] \qquad (\gamma > 0)\,, \tag{9}$$

where we have defined

$$\gamma = \sqrt{\frac{\Delta t}{8}\frac{m^2}{g}}\,, \tag{10}$$

and $K_\alpha(z)$ is the modified Bessel function of the second kind. Note that (9) only applies for positive mass squared. For $m^2 < 0$ we must analytically continue the Bessel function arguments in a full circle around the origin [1]. Remembering to now include the constant term in (8), one arrives at

$$\frac{\langle S_0 \rangle}{N} = \frac{1}{4} + \gamma^2 \left[1 - \frac{K_{3/4}(\gamma^2) + \sqrt{2}\pi I_{3/4}(\gamma^2)}{K_{1/4}(\gamma^2) + \sqrt{2}\pi I_{1/4}(\gamma^2)} \right] \qquad (\gamma < 0)\,. \tag{11}$$

The full function is plotted in Figure 1. Notice the asymptotes to $\frac{1}{2}$ for both positive and negative mass squared, as the theory becomes free (quadratic) about its minima. The minimum near $m^2 = 0$ is when the potential is most "boxy". Interestingly, as m^2 decreases further the function briefly rises above its free value, due to the particle spending an inordinate time straddling the ridge between the two VEVs.

This toy model will turn out to describe the full theory (including kinetic term) quite well in this respect.

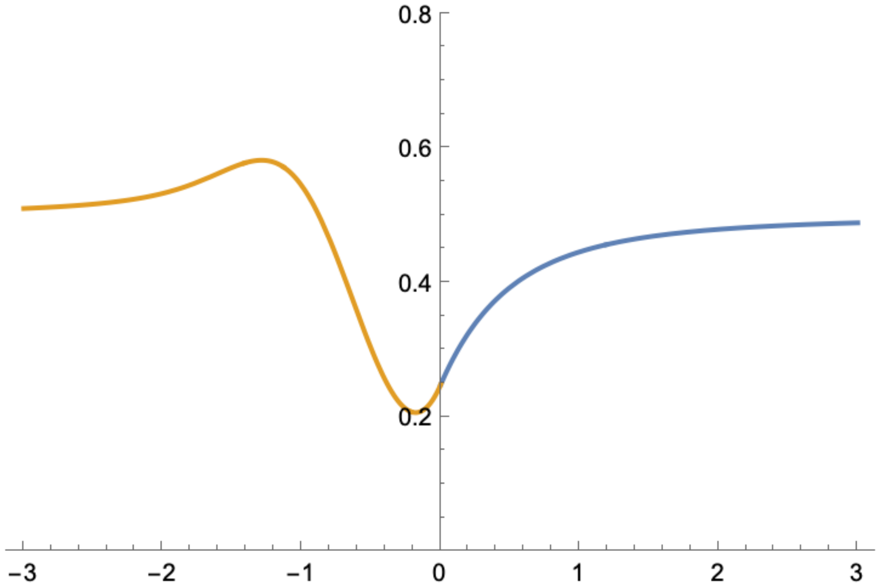

Figure 1: The action per lattice site $\langle S_0 \rangle / N$ as a function of γ, for the toy model (8).

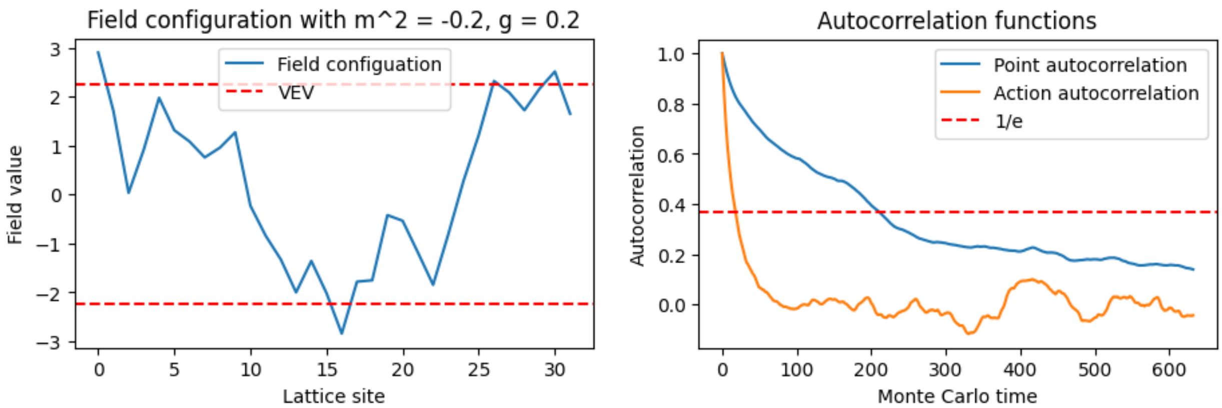

Figure 2: (Left) An instanton-anti-instanton configuration. (Right) The autocorrelation functions of the field value at a point and of the action. The autocorrelation time is when they cross below $1/e$. Notice how the action becomes uncorrelated from itself after many fewer Monte Carlo steps than the field at any given point.

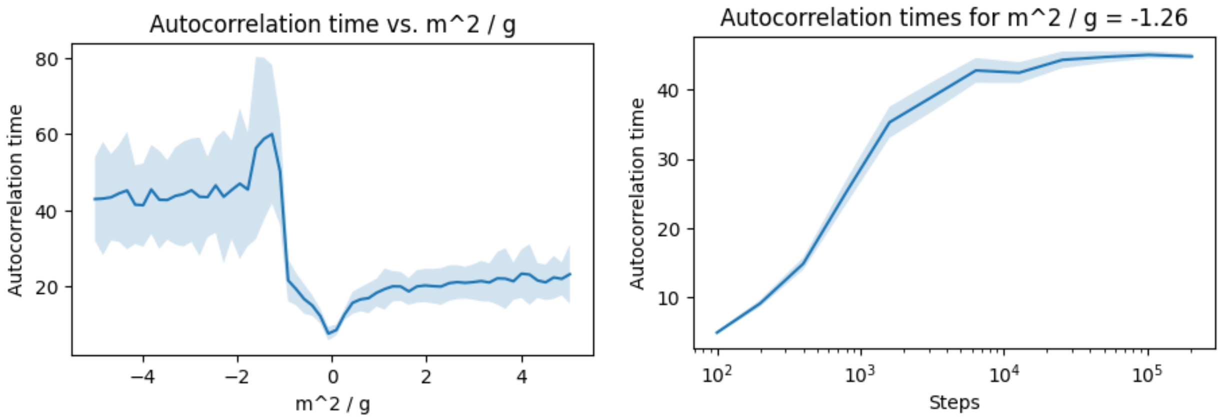

Figure 3: (Left) The autocorrelation time of the action for a range of couplings ($\Delta t = 1$). The discontinuity at -1 is due to different Monte Carlo sampling. On the left the noise is peaked at lattice sites in order to have the best chance at crossing over the potential barrier, while on the right the noise is distributed uniformly across the lattice. (Right) The autocorrelation time saturates, even at the maximum of the plot on the left, after allowing $\mathcal{O}(10^4)$ time steps. This indicates that the simulation truly does explore the distribution of actions.

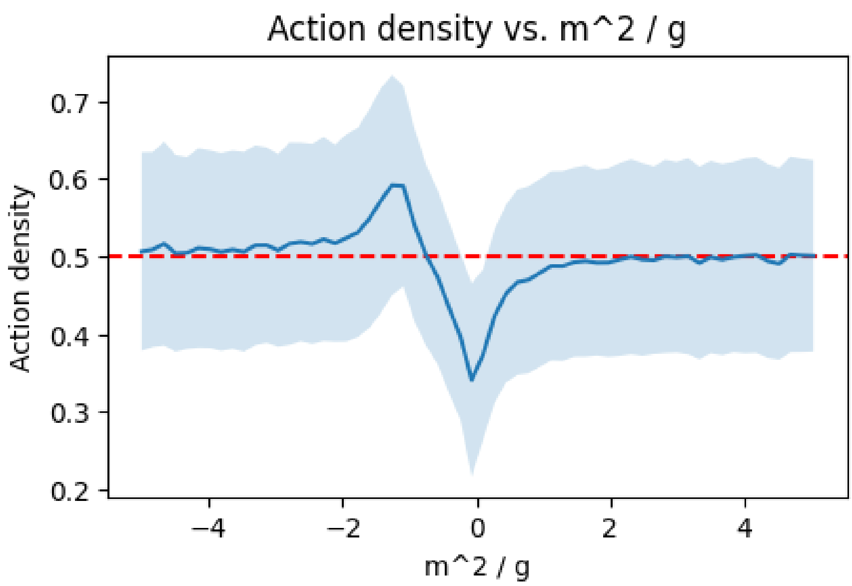

Figure 4: The action per lattice site ($\Delta t = 1$). Notice the similarity to Figure 1, besides the significantly different horizontal axis scaling (remember the factor of $\sqrt{8}$).

3 The Dynamical Theory

References

[1] "*NIST Digital Library of Mathematical Functions*." https://dlmf.nist.gov/, release 1.2.3 of 2024-12-15. https://dlmf.nist.gov/10.34.E2. F. W. J. Olver, A. B. Olde Daalhuis, D. W. Lozier, B. I. Schneider, R. F. Boisvert, C. W. Clark, B. R. Miller, B. V. Saunders, H. S. Cohl, and M. A. McClain, eds.